



INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

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| <p>(51) International Patent Classification ⁶ : C07D 471/04, 473/00, A61K 31/505, 31/535 // (C07D 471/04, 235:00, 221:00)</p> | <p>A1</p> | <p>(11) International Publication Number: WO 99/01454 (43) International Publication Date: 14 January 1999 (14.01.99)</p> |
| <p>(21) International Application Number: PCT/US98/13913 (22) International Filing Date: 2 July 1998 (02.07.98) (30) Priority Data: 60/051,628 3 July 1997 (03.07.97) US 60/080,665 3 April 1998 (03.04.98) US (71) Applicant: DU PONT PHARMACEUTICALS COMPANY [US/US]; 1007 Market Street, Wilmington, DE 19898 (US). (72) Inventors: WILDE, Richard, G.; 205 Roseman Court, Newark, DE 19711 (US). BAKTHAVATCHALAM, Rajagopal; 125 Berry Drive, Wilmington, DE 19808 (US). BECK, James, P.; 983 Tamara Drive, Smyrna, DE 19977 (US). ARVANI- TIS, Argyrios, G.; 101 Willow Glen Drive, Kennett Square, PA 19348 (US). (74) Agent: O'BRIEN, Maureen; Du Pont Pharmaceuticals Com- pany, Legal Patent Records Center, 1007 Market Street, Wilmington, DE 19898 (US).</p> | | <p>(81) Designated States: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE). Published With international search report.</p> |
| <p>(54) Title: IMIDAZOPYRIMIDINES AND IMIDAZOPYRIDINES FOR THE TREATMENT OF NEUROLOGICAL DISORDERS</p> <div style="text-align: center;"> <p>(I)</p> </div> <p>(57) Abstract</p> <p>Corticotropin releasing factor (CRF) antagonists of formula (I) and their use in treating psychiatric disorders and neurological diseases, anxiety-related disorders, post-traumatic stress disorder, supranuclear palsy and feeding disorders as well as treatment of immunological, cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathological disturbance and stress in mammals.</p> | | |

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TITLE

IMIDAZOPYRIMIDINES AND IMIDAZOPYRIDINES FOR THE TREATMENT
OF NEUROLOGICAL DISORDERS

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FIELD OF THE INVENTION

The present invention relates to novel compounds, compositions, and methods for the treatment of psychiatric disorders and neurological diseases, including major depression, anxiety-related disorders, post-traumatic stress disorder, supranuclear palsy and feeding disorders, as well as treatment of immunological, cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathological disturbance and stress.

10 In particular, the present invention relates to novel imidazopyrimidines and imidazopyridines, pharmaceutical compositions containing such compounds and their use in treating psychiatric disorders, neurological diseases, immunological, cardiovascular or heart-related diseases and

15 colonic hypersensitivity associated with psychopathological disturbance and stress.

20

BACKGROUND OF THE INVENTION

Corticotropin releasing factor (herein referred to as CRF), a 41 amino acid peptide, is the primary physiological regulator of proopiomelanocortin (POMC) -derived peptide secretion from the anterior pituitary gland [J. Rivier et al., *Proc. Nat. Acad. Sci. (USA)* 80:4851 (1983); W. Vale et al., *Science* 213:1394 (1981)]. In addition to its endocrine

25 role at the pituitary gland, immunohistochemical localization of CRF has demonstrated that the hormone has a broad extrahypothalamic distribution in the central nervous system and produces a wide spectrum of autonomic, electrophysiological and behavioral effects consistent with

30 a neurotransmitter or neuromodulator role in brain [W. Vale et al., *Rec. Prog. Horm. Res.* 39:245 (1983); G.F. Koob, *Persp. Behav. Med.* 2:39 (1985); E.B. De Souza et al., *J. Neurosci.* 5:3189 (1985)]. There is also evidence that CRF

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plays a significant role in integrating the response of the immune system to physiological, psychological, and immunological stressors [J.E. Blalock, *Physiological Reviews* 69:1 (1989); J.E. Morley, *Life Sci.* 41:527 (1987)].

Clinical data provide evidence that CRF has a role in psychiatric disorders and neurological diseases including depression, anxiety-related disorders and feeding disorders. A role for CRF has also been postulated in the etiology and pathophysiology of Alzheimer's disease, Parkinson's disease, Huntington's disease, progressive supranuclear palsy and amyotrophic lateral sclerosis as they relate to the dysfunction of CRF neurons in the central nervous system [for review see E.B. De Souza, *Hosp. Practice* 23:59 (1988)].

In affective disorder, or major depression, the concentration of CRF is significantly increased in the cerebral spinal fluid (CSF) of drug-free individuals [C.B. Nemeroff et al., *Science* 226:1342 (1984); C.M. Banki et al., *Am. J. Psychiatry* 144:873 (1987); R.D. France et al., *Biol. Psychiatry* 28:86 (1988); M. Arato et al., *Biol Psychiatry* 25:355 (1989)]. Furthermore, the density of CRF receptors is significantly decreased in the frontal cortex of suicide victims, consistent with a hypersecretion of CRF [C.B. Nemeroff et al., *Arch. Gen. Psychiatry* 45:577 (1988)]. In addition, there is a blunted adrenocorticotropin (ACTH) response to CRF (i.v. administered) observed in depressed patients [P.W. Gold et al., *Am J. Psychiatry* 141:619 (1984); F. Holsboer et al., *Psychoneuroendocrinology* 9:147 (1984); P.W. Gold et al., *New Eng. J. Med.* 314:1129 (1986)]. Preclinical studies in rats and non-human primates provide additional support for the hypothesis that hypersecretion of CRF may be involved in the symptoms seen in human depression [R.M. Sapolsky, *Arch. Gen. Psychiatry* 46:1047 (1989)]. There is preliminary evidence that tricyclic antidepressants can alter CRF levels and thus modulate the numbers of CRF receptors in

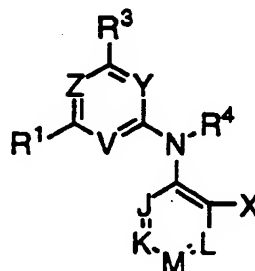
brain [Grigoriadis et al., *Neuropsychopharmacology* 2:53 (1989)].

It has also been postulated that CRF has a role in the etiology of anxiety-related disorders. CRF produces
5 anxiogenic effects in animals and interactions between benzodiazepine / non-benzodiazepine anxiolytics and CRF have been demonstrated in a variety of behavioral anxiety models [D.R. Britton et al., *Life Sci.* 31:363 (1982); C.W. Berridge and A.J. Dunn *Regul. Peptides* 16:83 (1986)].
10 Preliminary studies using the putative CRF receptor antagonist α -helical ovine CRF (9-41) in a variety of behavioral paradigms demonstrate that the antagonist produces "anxiolytic-like" effects that are qualitatively similar to the benzodiazepines [C.W. Berridge and A.J. Dunn
15 *Horm. Behav.* 21:393 (1987), *Brain Research Reviews* 15:71 (1990)].

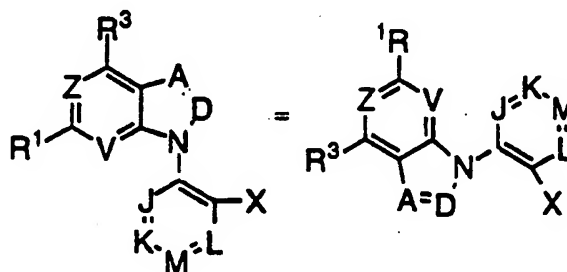
Neurochemical, endocrine and receptor binding studies have all demonstrated interactions between CRF and benzodiazepine anxiolytics, providing further evidence for
20 the involvement of CRF in these disorders. Chlordiazepoxide attenuates the "anxiogenic" effects of CRF in both the conflict test [K.T. Britton et al., *Psychopharmacology* 86:170 (1985); K.T. Britton et al., *Psychopharmacology* 94:306 (1988)] and in the acoustic startle test [N.R.
25 Swerdlow et al., *Psychopharmacology* 88:147 (1986)] in rats. The benzodiazepine receptor antagonist (Ro15-1788), which was without behavioral activity alone in the operant conflict test, reversed the effects of CRF in a dose-dependent manner while the benzodiazepine inverse agonist
30 (FG7142) enhanced the actions of CRF [K.T. Britton et al., *Psychopharmacology* 94:306 (1988)].

It has been further postulated that CRF has a role in immunological, cardiovascular or heart-related diseases such as hypertension, tachycardia and congestive heart
35 failure, stroke, osteoporosis, premature birth, psychosocial dwarfism, stress-induced fever, ulcer, diarrhea, post-operative ileus and colonic hypersensitivity associated with psychopathological disturbance and stress.

- The mechanisms and sites of action through which the standard anxiolytics and antidepressants produce their therapeutic effects remain to be elucidated. It has been hypothesized however, that they are involved in the suppression of the CRF hypersecretion that is observed in these disorders. Of particular interest is that preliminary studies examining the effects of a CRF receptor antagonist (a-helical CRF9-41) in a variety of behavioral paradigms have demonstrated that the CRF antagonist produces "anxiolytic-like" effects qualitatively similar to the benzodiazepines [for review see G.F. Koob and K.T. Britton, In: *Corticotropin-Releasing Factor: Basic and Clinical Studies of a Neuropeptide*, E.B. De Souza and C.B. Nemeroff eds., CRC Press p221 (1990)].
- DuPont Merck PCT application US94/11050 describes corticotropin releasing factor antagonist compounds of the formula:



- and their use to treat psychiatric disorders and neurological diseases. Included in the description are fused pyridines and pyrimidines of the formula:



- where: V is CR^{1a} or N; Z is CR² or N; A is CR³ or N; and D is CR²⁸ or N.

Other compounds reported to have activity as corticotropin releasing factors are disclosed in WO 95/33750, WO 95/34563 and WO 95/33727.

5

SUMMARY OF THE INVENTION

In accordance with one aspect, the present invention provides novel compounds which bind to corticotropin releasing factor receptors, thereby altering the anxiogenic effects of CRF secretion. The compounds of the present invention are useful for the treatment of psychiatric disorders and neurological diseases, anxiety-related disorders, post-traumatic stress disorder, supranuclear palsy and feeding disorders as well as treatment of immunological, cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathological disturbance and stress in mammals.

20 According to another aspect, the present invention provides novel compounds of formula (I) (described below) which are useful as antagonists of the corticotropin releasing factor. The compounds of the present invention exhibit activity as corticotropin releasing factor
25 antagonists and appear to suppress CRF hypersecretion. The present invention also includes pharmaceutical compositions containing such compounds of formula (I), and methods of using such compounds for the suppression of CRF hypersecretion, and/or for the treatment of anxiogenic
30 disorders.

According to yet another aspect, the present invention provides novel compounds, pharmaceutical compositions and methods which may be used in the treatment of affective
35 disorder, anxiety, depression, irritable bowel syndrome, post-traumatic stress disorder, supranuclear palsy, immune suppression, Alzheimer's disease, gastrointestinal disease, anorexia nervosa or other feeding disorder, drug or alcohol

withdrawal symptoms, drug addiction, inflammatory disorder, fertility problems, disorders, the treatment of which can be effected or facilitated by antagonizing CRF, including but not limited to disorders induced or facilitated by CRF, or a disorder selected from inflammatory disorders such as rheumatoid arthritis and osteoarthritis, pain, asthma, psoriasis and allergies; generalized anxiety disorder; panic, phobias, obsessive-compulsive disorder; post-traumatic stress disorder; sleep disorders induced by stress; pain perception such as fibromyalgia; mood disorders such as depression, including major depression, single episode depression, recurrent depression, child abuse induced depression, and postpartum depression; dysthemia; bipolar disorders; cyclothymia; fatigue syndrome; stress-induced headache; cancer, human immunodeficiency virus (HIV) infections; neurodegenerative diseases such as Alzheimer's disease, Parkinson's disease and Huntington's disease; gastrointestinal diseases such as ulcers, irritable bowel syndrome, Crohn's disease, spastic colon, diarrhea, and post operative ileus and colonic hypersensitivity associated by psychopathological disturbances or stress; eating disorders such as anorexia and bulimia nervosa; hemorrhagic stress; stress-induced psychotic episodes; euthyroid sick syndrome; syndrome of inappropriate antidiarrhetic hormone (ADH); obesity; infertility; head traumas; spinal cord trauma; ischemic neuronal damage (e.g., cerebral ischemia such as cerebral hippocampal ischemia); excitotoxic neuronal damage; epilepsy; cardiovascular and hear related disorders including hypertension, tachycardia and congestive heart failure; stroke; immune dysfunctions including stress induced immune dysfunctions (e.g., stress induced fevers, porcine stress syndrome, bovine shipping fever, equine paroxysmal fibrillation, and dysfunctions induced by confinement in chickens, sheering stress in sheep or human-animal interaction related stress in dogs); muscular spasms; urinary incontinence; senile dementia of the Alzheimer's type; multiinfarct dementia; amyotrophic

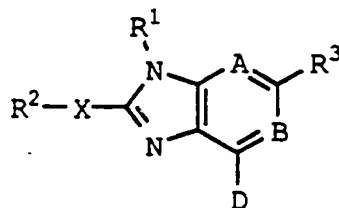
lateral sclerosis; chemical dependencies and addictions
(e.g., dependencies on alcohol, cocaine, heroin,
benzodiazepines, or other drugs); drug and alcohol
withdrawal symptoms; osteoporosis; psychosocial dwarfism
5 and hypoglycemia in mammals.

According to a still further aspect of the invention,
the compounds provided by this invention (and especially
labelled compounds of this invention) are also useful as
10 standards and reagents in determining the ability of a
potential pharmaceutical to bind to the CRF receptor.

DETAILED DESCRIPTION OF INVENTION

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[1] Thus, in a first embodiment, the present invention
provides a novel compound of formula I:



20

(I)

or a stereoisomer or pharmaceutically acceptable salt form
thereof, wherein:

A is N or C-R⁷;

25

B is N or C-R⁸;

provided that at least one of the groups A and B is N;

30 D is an aryl or heteroaryl group attached through an
unsaturated carbon atom;

X is selected from the group CH-R⁹, N-R¹⁰, O, S(O)_n and a
bond;

n is 0, 1 or 2;

5 R^1 is selected from the group C₁₋₁₀ alkyl, C₂₋₁₀ alkenyl, C₂₋₁₀ alkynyl, C₃₋₈ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, -SO₂-C₁₋₁₀ alkyl, -SO₂-R^{1a}, and -SO₂-R^{1b};

10 R^1 is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b}, -CONR^{13a}R^{16a}, 1-morpholinyl, 1-piperidinyl, 1-piperazinyl, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group
15 selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-, and wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

20 R^1 is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, R^{1c}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₄ alkoxy-C₁₋₄ alkyl, and C₃₋₈ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is
25 replaced by -O-;

provided that R¹ is other than:

- 30 (a) a cyclohexyl-(CH₂)₂- group;
(b) a 3-cyclopropyl-3-methoxypropyl group;
(c) an unsubstituted-(alkoxy)methyl group; and,
(d) a 1-hydroxyalkyl group;

35 also provided that when R¹ alkyl substituted with OH, then the carbon adjacent to the ring N is other than CH₂;

- R^{1a} is aryl and is selected from the group phenyl, naphthyl, indanyl and indenyl, each R^{1a} being substituted with 0-1 $-OR^{17}$ and 0-5 substituents independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, -CN, nitro, SH, $-S(O)_nR^{18}$, $-COR^{17}$, $-OC(O)R^{18}$, $-NR^{15a}COR^{17}$, $-N(COR^{17})_2$, $-NR^{15a}CONR^{17a}R^{19a}$, $-NR^{15a}CO_2R^{18}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$;
- R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-onyl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, -CN, nitro, $-OR^{17}$, SH, $-S(O)_nR^{18}$, $-COR^{17}$, $-OC(O)R^{18}$, $-NR^{15a}COR^{17}$, $-N(COR^{17})_2$, $-NR^{15a}CONR^{17a}R^{19a}$, $-NR^{15a}CO_2R^{18}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15a} , CO_2R^{14b} , COR^{14b} and SO_2R^{14b} ;
- R^{1c} is heterocyclyl and is a saturated or partially saturated heteroaryl, each heterocyclyl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, -CN, nitro, $-OR^{13a}$, SH, $-S(O)_nR^{14b}$, $-COR^{13a}$, $-OC(O)R^{14b}$, $-NR^{15a}COR^{13a}$, $-N(COR^{13a})_2$, $-NR^{15a}CONR^{13a}R^{16a}$,

5 $-\text{NR}^{15\text{a}}\text{CO}_2\text{R}^{14\text{b}}$, $-\text{NR}^{13\text{a}}\text{R}^{16\text{a}}$, and $-\text{CONR}^{13\text{a}}\text{R}^{16\text{a}}$ and each heterocyclyl being substituted on any nitrogen atom with 0-1 substituents selected from the group $\text{R}^{13\text{a}}$, $\text{CO}_2\text{R}^{14\text{b}}$, $\text{COR}^{14\text{b}}$ and $\text{SO}_2\text{R}^{14\text{b}}$ and wherein any sulfur atom is optionally monooxidized or dioxidized;

10 provided that R^1 is other than a $-(\text{CH}_2)_{1-4}\text{-aryl}$, $-(\text{CH}_2)_{1-4}\text{-heteroaryl}$, or $-(\text{CH}_2)_{1-4}\text{-heterocycle}$, wherein the aryl, heteroaryl, or heterocycle group is substituted or unsubstituted;

15 R^2 is selected from the group C_{1-4} alkyl, C_{3-8} cycloalkyl, C_{2-4} alkenyl, and C_{2-4} alkynyl and is substituted with 0-3 substituents selected from the group $-\text{CN}$, hydroxy, halo and C_{1-4} alkoxy;

 alternatively R^2 , in the case where X is a bond, is selected from the group $-\text{CN}$, CF_3 and C_2F_5 ;

20 R^3 , R^7 and R^8 are independently selected at each occurrence from the group H, Br, Cl, F, I, $-\text{CN}$, C_{1-4} alkyl, C_{3-8} cycloalkyl, C_{1-4} alkoxy, C_{1-4} alkylthio, C_{1-4} alkylsulfinyl, C_{1-4} alkylsulfonyl, amino, C_{1-4} alkylamino, $(\text{C}_{1-4} \text{ alkyl})_2\text{amino}$ and phenyl, each phenyl is substituted with 0-3 groups selected from the group

25 C_{1-7} alkyl, C_{3-8} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, nitro, C_{1-4} alkoxy, C_{1-4} haloalkoxy, C_{1-4} alkylthio, C_{1-4} alkyl sulfinyl, C_{1-4} alkylsulfonyl, C_{1-6} alkylamino and $(\text{C}_{1-4} \text{ alkyl})_2\text{amino}$;

30 provided that when R^1 is unsubstituted C_{1-10} alkyl, then R^3 is other than substituted or unsubstituted phenyl;

35 R^9 and R^{10} are independently selected at each occurrence from the group H, C_{1-4} alkyl, C_{3-6} cycloalkyl- C_{1-4} alkyl and C_{3-8} cycloalkyl;

R¹³ is selected from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)-;

5

R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

10

R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)- and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy C₁₋₄ haloalkoxy, and dimethylamino;

15

20 R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

25

30 R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

30

R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

35

R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

5

R¹⁷ is selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₁₋₄ haloalkyl, R¹⁴S(O)_n-C₁₋₄ alkyl, and R^{17b}R^{19b}N-C₂₋₄ alkyl;

10

R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;

15

alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;

20

alternatively, in an NR^{17b}R^{19b} moiety, R^{17b} and R^{19b} taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;

25

R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ haloalkyl;

30

aryl is independently selected at each occurrence from the group phenyl, naphthyl, indanyl and indenyl, each aryl being substituted with 0-5 substituents independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, methylenedioxy, C₁₋₄ alkoxy-C₁₋₄ alkoxy, -OR¹⁷, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, -NO₂,

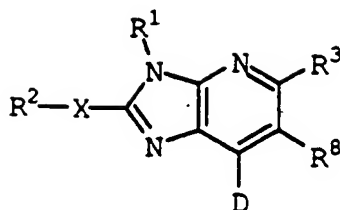
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SH, $-S(O)_nR^{18}$, $-COR^{17}$, $-CO_2R^{17}$, $-OC(O)R^{18}$, $-NR^{15}COR^{17}$,
 $-N(COR^{17})_2$, $-NR^{15}CONR^{17}R^{19}$, $-NR^{15}CO_2R^{18}$, $-NR^{17}R^{19}$, and
 $-CONR^{17}R^{19}$ and up to 1 phenyl, each phenyl substituent
 5 being substituted with 0-4 substituents selected from
 the group C_{1-3} alkyl, C_{1-3} alkoxy, Br, Cl, F, I, -CN,
 dimethylamino, CF_3 , C_2F_5 , OCF_3 , SO_2Me and acetyl;

heteroaryl is independently selected at each occurrence from
 the group pyridyl, pyrimidinyl, triazinyl, furanyl,
 10 quinolinyl, isoquinolinyl, thienyl, imidazolyl,
 thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl,
 benzothienyl, benzothiazolyl, benzoxazolyl,
 isoxazolyl, triazolyl, tetrazolyl, indazolyl,
 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl,
 15 2,3-dihydrobenzothienyl-S-oxide,
 2,3-dihydrobenzothienyl-S-dioxide, indolinyl,
 benzoxazolin-2-on-yl, benzodioxolanyl and
 benzodioxane, each heteroaryl being substituted 0-4
 carbon atoms with a substituent independently selected
 20 at each occurrence from the group C_{1-6} alkyl, C_{3-6}
 cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, -CN, nitro,
 $-OR^{17}$, SH, $-S(O)_mR^{18}$, $-COR^{17}$, $-CO_2R^{17}$, $-OC(O)R^{18}$,
 $-NR^{15}COR^{17}$, $-N(COR^{17})_2$, $-NR^{15}CONR^{17}R^{19}$, $-NR^{15}CO_2R^{18}$,
 $-NR^{17}R^{19}$, and $-CONR^{17}R^{19}$ and each heteroaryl being
 25 substituted on any nitrogen atom with 0-1 substituents
 selected from the group R^{15} , CO_2R^{14a} , COR^{14a} and
 SO_2R^{14a} ; and,

provided that when D is imidazole or triazole, R^1 is other
 30 than unsubstituted C_{1-6} linear or branched alkyl or
 C_{3-6} cycloalkyl.

[2] In a preferred embodiment, the present invention provides
 35 a novel compound of formula Ia:



(Ia).

- 5 [2a] In a more preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

X is selected from the group O, S(O)_n and a bond;

- 10 n is 0, 1 or 2;

R¹ is selected from the group C₁₋₆ alkyl, C₂₋₆ alkenyl, C₂₋₆ alkynyl, and C₃₋₈ cycloalkyl;

- 15 R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and
20 -NSO₂R^{14b}-;

- R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃,
25 CF₂CF₃, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₈ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

- 30 provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;

R^{1a} is aryl and is selected from the group phenyl and indanyl, each R^{1a} being substituted with 0-1 -OR¹⁷ and 0-5 substituents independently selected at each

occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a};

- 5 R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, furanyl, thienyl, imidazolyl, thiazolyl, pyrrolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-4 carbon atoms with a substituent
10 independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, CF₃, -CN, -OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a} and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group
15 R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

provided that R¹ is other than a -(CH₂)₁₋₄-aryl or -(CH₂)₁₋₄-heteroaryl wherein the aryl or heteroaryl group is substituted or unsubstituted;

- 20 R² is selected from the group C₁₋₄ alkyl, C₂₋₄ alkenyl, and C₂₋₄ alkynyl and is substituted with 0-1 substituents selected from the group -CN, OH, Cl, F, and C₁₋₄ alkoxy;

- 25 R³ and R⁸ are independently selected at each occurrence from the group H, Br, Cl, F, -CN, C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₁₋₄ alkoxy, NH₂, C₁₋₄ alkylamino, and (C₁₋₄ alkyl)₂-amino;

- 30 R⁹ is independently selected at each occurrence from the group H, C₁₋₄ alkyl and C₃₋₈ cycloalkyl;

- 35 R¹³ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;

- R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 5 R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;
- 10 R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;
- R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;
- 15 R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, C₁₋₄ haloalkyl, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;
- 20 R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 25 R¹⁷, R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;
- 30 alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in
- 35

1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13} , CO_2R^{14} , COR^{14} and SO_2R^{14} ;

5 R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C_{1-6} alkyl, C_{3-10} cycloalkyl, C_{3-6} cycloalkyl- C_{1-6} alkyl and C_{1-4} haloalkyl;

10 aryl is phenyl substituted with 1-4 substituents independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, $-OR^{17}$, Br, Cl, F, C_{1-4} haloalkyl, $-CN$, $-S(O)_nR^{18}$, $-COR^{17}$, $-CO_2R^{17}$, $-NR^{15}COR^{17}$, $-NR^{15}CO_2R^{18}$, $-NR^{17}R^{19}$, and $-CONR^{17}R^{19}$; and,

15 heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, tetrazolyl, indazolyl,
20 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 1-4
25 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, C_{1-4} haloalkyl, $-CN$, $-OR^{17}$, $-S(O)_mR^{18}$, $-COR^{17}$, $-CO_2R^{17}$, $-OC(O)R^{18}$, $-NR^{15}COR^{17}$, $-N(COR^{17})_2$, $-NR^{15}CO_2R^{18}$, $-NR^{17}R^{19}$, and $-CONR^{17}R^{19}$ and
30 each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15} , CO_2R^{14a} , COR^{14a} and SO_2R^{14a} .

35 [2b] In an even more preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

X is selected from the group O, S and a bond;

R¹ is substituted C₁₋₆ alkyl;

- 5 R¹ is substituted with 0-1 substituents selected from the group -CN, -CO₂R^{13a}, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;

10

- R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl which is substituted with 0-1 CH₃ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

15

provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;

20

- R^{1a} is aryl and is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-3 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂;

25

- R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen

30

35

atom with 0-1 substituents selected from the group
CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

provided that R¹ is other than a -(CH₂)₁₋₄-aryl or
5 -(CH₂)₁₋₄-heteroaryl wherein the aryl or heteroaryl
group is substituted or unsubstituted;

R² is selected from the group CH₃, CH₂CH₃, CH(CH₃)₂, and
CH₂CH₂CH₃;

10

R³ and R⁸ are independently selected at each occurrence from
the group H, CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

aryl is phenyl substituted with 2-4 substituents
15 independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl,
OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F,
CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,
-C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

20

heteroaryl is independently selected at each occurrence from
the group pyridyl, indolyl, benzothienyl,
2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl,
2,3-dihydrobenzothienyl-S-oxide,

25 2,3-dihydrobenzothienyl-S-dioxide, indoliny, and
benzoxazolin-2-on-yl, each heteroaryl being
substituted on 2-4 carbon atoms with a substituent
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl,
30 OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F,
CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,
-C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each
heteroaryl being substituted on any nitrogen atom with
0-1 substituents selected from the group CH₃, CO₂CH₃,
35 COCH₃ and SO₂CH₃.

[2c] In a still more preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

R¹ is substituted C₁;

5

R¹ is substituted with 0-1 substituents selected from the group -CN, -CO₂CH₃, and -CO₂CH₂CH₃;

10 R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃, F, CF₃, cyclopropyl, CH₃-cyclopropyl, cyclobutyl, CH₃-cyclobutyl, cyclopentyl, CH₃-cyclopentyl;

15

R^{1a} is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, and OCF₃, and 0-2 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃,
20 -CN, and SCH₃;

20

R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, and tetrazolyl, each heteroaryl
25 being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, and SCH₃ and each heteroaryl being substituted on any nitrogen atom with
30 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

30

provided that R¹ is other than a -(CH₂)₁₋₄-aryl or -(CH₂)₁₋₄-heteroaryl wherein the aryl or heteroaryl
35 group is substituted or unsubstituted;

35

R² is selected from the group CH₃, CH₂CH₃, and CH(CH₃)₂;

R³ and R⁸ are independently selected at each occurrence from the group H and CH₃;

aryl is phenyl substituted with 2-4 substituents
5 independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

10 heteroaryl is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂,
15 OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂.

20 [2d] In a further preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

R¹ is substituted (cyclopropyl)-C₁ alkyl or (cyclobutyl)-C₁ alkyl;

25 R¹ is substituted with 0-1 -CN;

R¹ is also substituted with 0-1 substituents independently
30 selected at each occurrence from the group R^{1a}, R^{1b}, CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃, F, CF₃, cyclopropyl, and CH₃-cyclopropyl;

35 R^{1a} is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, and OCF₃, and 0-2 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃, -CN, and SCH₃;

5 R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, and pyrazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $CH_2CH_2CH_3$, OCH_3 , OCH_2CH_3 , OCF_3 , Br, Cl, F, CF_3 , -CN, and SCH_3 .

10

[2e] In another further preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

15 R^1 is (cyclopropyl) C_1 alkyl or (cyclobutyl)- C_1 alkyl substituted with 1 substituent independently selected at each occurrence from the group R^{1a} , R^{1b} , CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $CH_2CH_2CH_3$, $-(CH_2)_3CH_3$, $-CH=CH_2$, $-CH=CH(CH_3)$, $-CH\equiv CH$, $-CH\equiv C(CH_3)$, $-CH_2OCH_3$, $-CH_2CH_2OCH_3$, F, CF_3 , cyclopropyl, and CH_3 -cyclopropyl;

20

R^{1a} is phenyl substituted with 0-2 substituents independently selected at each occurrence from the group CH_3 , CH_2CH_3 , Cl, F, and CF_3 ;

25 R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, and isoxazolyl, each heteroaryl being substituted on 0-2 carbon atoms with a substituent independently selected at each occurrence from the group CH_3 , OCH_3 , Cl, F, and CF_3 .

30

[2f] In an even further preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

35 R^1 is selected from the group (cyclopropyl) $CH-CH_3$, (cyclopropyl) $CH-CH_2CH_3$, (cyclopropyl) $CH-CH_2OCH_3$, (cyclopropyl) $CH-CH_2CH_2CH_3$, (cyclopropyl) $CH-CH_2CH_2OCH_3$, (cyclopropyl) $_2CH$, phenyl(cyclopropyl) CH ,

furanyl(cyclopropyl)CH, thienyl(cyclopropyl)CH,
isoxazolyl(cyclopropyl)CH, (CH₃-
furanyl)(cyclopropyl)CH, (cyclobutyl)CH-CH₃,
(cyclobutyl)CH-CH₂CH₃, (cyclobutyl)CH-CH₂OCH₃,
5 (cyclobutyl)CH-CH₂CH₂CH₃, (cyclobutyl)CH-CH₂CH₂OCH₃,
(cyclobutyl)₂CH, phenyl(cyclobutyl)CH,
furanyl(cyclobutyl)CH, thienyl(cyclobutyl)CH,
isoxazolyl(cyclobutyl)CH, and (CH₃-
furanyl)(cyclobutyl)CH;
10

[2g] In another further preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

15 D is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

20

[2h] In another further preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

D is pyridyl substituted on 2-4 carbon atoms with a
25 substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

30

[2i] In another preferred embodiment, the present invention provides a novel compound of formula Ia, wherein the compound is selected from the group:

35 3-(1-cyclopropylpropyl)-7-(2,4-dichlorophenyl)-2-ethyl-3H-imidazo[4,5-b]pyridine;

- 3-(1-cyclopropylpropyl)-7-(2,4-dichlorophenyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 3-(1-cyclopropylpropyl)-7-(2,4-dichlorophenyl)-2-(methysulfanyl)-3H-imidazo[4,5-b]pyridine;
- 7-[2-chloro-4-(trifluoromethyl)phenyl]-3-(1-cyclopropylpropyl)-2-ethyl-3H-imidazo[4,5-b]pyridine;
- 10 7-[2-chloro-4-(trifluoromethyl)phenyl]-3-(1-cyclopropylpropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 7-[2-chloro-4-(trifluoromethyl)phenyl]-3-(1-cyclopropylpropyl)-2-(methysulfanyl)-3H-imidazo[4,5-b]pyridine;
- 15 b]pyridine;
- 3-(1-cyclopropylpropyl)-2-ethyl-7-[2-methyl-4-(trifluoromethyl)phenyl]-3H-imidazo[4,5-b]pyridine;
- 20 7-(2-chloro-4-methoxyphenyl)-3-(1-cyclopropylpropyl)-2-ethyl-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-4-methoxyphenyl)-3-(1-cyclopropylpropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 25 3-(1-cyclopropylpropyl)-2-ethyl-7-(4-methoxy-2,5-dimethylphenyl)-3H-imidazo[4,5-b]pyridine;
- 3-(1-cyclopropylpropyl)-2-methoxy-7-(4-methoxy-2,5-dimethylphenyl)-3H-imidazo[4,5-b]pyridine;
- 30 7-(2-chloro-4-methoxyphenyl)-3-(1-cyclopropylpropyl)-2-ethyl-3H-imidazo[4,5-b]pyridine;
- 35 7-(2-chloro-4-methoxyphenyl)-3-(1-cyclopropylpropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;

- 7-(2-chloro-5-fluoro-4-methoxyphenyl)-3-(1-cyclopropylpropyl)-
2-ethyl-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-fluoro-4-methoxyphenyl)-3-(1-cyclopropylpropyl)-2-
5 methoxy-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-5-fluoro-4-methylphenyl)-3-(1-cyclopropylpropyl)-
2-ethyl-3H-imidazo[4,5-b]pyridine;
- 10 7-(2-chloro-fluoro-4-methylphenyl)-3-(1-cyclopropylpropyl)-2-
methoxy-3H-imidazo[4,5-b]pyridine;
- 3-(1-cyclopropylpropyl)-2-ethyl-7-(2,4,5-trimethylphenyl)-3H-
imidazo[4,5-b]pyridine;
- 15 3-(1-cyclopropylpropyl)-2-methoxy-7-(2,4,5-trimethylphenyl)-
3H-imidazo[4,5-b]pyridine;
- 3-(1-cyclopropylpropyl)-2-ethyl-7-(2,5,6-trimethyl-3-
20 pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 3-(1-cyclopropylpropyl)-2-methoxy-7-(2,5,6-trimethyl-3-
pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 25 3-(1-cyclopropylpropyl)-7-(2,6-dimethyl-3-pyridinyl)-2-ethyl-
3H-imidazo[4,5-b]pyridine;
- 3-(1-cyclopropylpropyl)-7-(2,6-dimethyl-3-pyridinyl)-2-
methoxy-3H-imidazo[4,5-b]pyridine;
- 30 3-(1-cyclopropylpropyl)-7-(2,6-dimethoxy-3-pyridinyl)-2-ethyl-
3H-imidazo[4,5-b]pyridine;
- 7-(2,4-dichlorophenyl)-2-ethyl-3-(1-ethylpropyl)-3H-
35 imidazo[4,5-b]pyridine;
- 7-(2,4-dichlorophenyl)-3-(1-ethylpropyl)-2-methoxy-3H-
imidazo[4,5-b]pyridine;

- 7-[2-chloro-4-(trifluoromethyl)phenyl]-2-ethyl-3-(1-ethylpropyl)-3H-imidazo[4,5-b]pyridine;
- 5 7-[2-chloro-4-(trifluoromethyl)phenyl]-3-(1-ethylpropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 7-[2-chloro-4-(methylsulfonyl)phenyl]-2-ethyl-3-(1-ethylpropyl)-3H-imidazo[4,5-b]pyridine;
- 10 7-[2-chloro-4-(methylsulfonyl)phenyl]-3-(1-ethylpropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 2-ethyl-3-(1-ethylpropyl)-7-(4-methoxy-2,5-dimethylphenyl)-3H-imidazo[4,5-b]pyridine;
- 15 3-(1-ethylpropyl)-2-methoxy-7-(4-methoxy-2,5-dimethylphenyl)-3H-imidazo[4,5-b]pyridine;
- 20 7-(2-chloro-4-methoxyphenyl)-2-ethyl-3-(1-ethylpropyl)-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-4-methoxyphenyl)-3-(1-ethylpropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 25 2-ethyl-3-(1-ethylpropyl)-7-[4-methoxy-2-(trifluoromethyl)phenyl]-3H-imidazo[4,5-b]pyridine;
- 3-(1-ethylpropyl)-2-methoxy-7-[4-methoxy-2-(trifluoromethyl)phenyl]-3H-imidazo[4,5-b]pyridine;
- 30 7-(2,6-dimethoxy-3-pyridinyl)-2-ethyl-3-(1-ethylpropyl)-3H-imidazo[4,5-b]pyridine;
- 35 7-(2,6-dimethyl-3-pyridinyl)-2-ethyl-3-(1-ethylpropyl)-3H-imidazo[4,5-b]pyridine;

- 2-ethyl-3-(1-ethylpropyl)-7-(2,5,6-trimethyl-3-pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 2-ethyl-3-(1-ethylpropyl)-7-(5-fluoro-4-methoxy-2-methylphenyl)-3H-imidazo[4,5-b]pyridine;
- 3-(1-ethylpropyl)-7-(5-fluoro-4-methoxy-2-methylphenyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 3-chloro-4-[2-ethyl-3-(1-ethylpropyl)-3H-imidazo[4,5-b]pyridin-7-yl]benzonitrile;
- 3-chloro-4-[3-(1-ethylpropyl)-2-methoxy-3H-imidazo[4,5-b]pyridin-7-yl]benzonitrile;
- 1-{3-chloro-4-[2-ethyl-3-(1-ethylpropyl)-3H-imidazo[4,5-b]pyridin-7-yl]phenyl}-1-ethanone;
- 1-{3-chloro-4-[3-(1-ethylpropyl)-2-methoxy-3H-imidazo[4,5-b]pyridin-7-yl]phenyl}-1-ethanone;
- 3-(dicyclopropylmethyl)-2-ethyl-7-(5-fluoro-4-methoxy-2-methylphenyl)-3H-imidazo[4,5-b]pyridine;
- 3-(dicyclopropylmethyl)-7-(5-fluoro-4-methoxy-2-methylphenyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-4-methoxyphenyl)-3-(dicyclopropylmethyl)-2-ethyl-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-4-methoxyphenyl)-3-(dicyclopropylmethyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 7-(2,4-dichlorophenyl)-3-(dicyclopropylmethyl)-2-ethyl-3H-imidazo[4,5-b]pyridine;
- 7-(2,4-dichlorophenyl)-3-(dicyclopropylmethyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;

- 7-[2-chloro-4-(trifluoromethyl)phenyl]-3-(dicyclopropylmethyl)-2-ethyl-3H-imidazo[4,5-b]pyridine;
- 5 7-[2-chloro-4-(trifluoromethyl)phenyl]-3-(dicyclopropylmethyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 7-(2,4-dichlorophenyl)-2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridine;
- 10 7-(2,4-dichlorophenyl)-3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 15 7-[2-chloro-4-(trifluoromethyl)phenyl]-2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridine;
- 7-[2-chloro-4-(trifluoromethyl)phenyl]-3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 20 7-(2-chloro-4-methoxyphenyl)-2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-4-methoxyphenyl)-3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 25 7-(2-chloro-5-fluoro-4-methoxyphenyl)-2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-5-fluoro-4-methoxyphenyl)-3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 30 2-ethyl-3-(1-ethyl-3-methoxypropyl)-7-(4-methoxy-2,5-dimethylphenyl)-3H-imidazo[4,5-b]pyridine;
- 35 3-(1-ethyl-3-methoxypropyl)-2-methoxy-7-(4-methoxy-2,5-dimethylphenyl)-3H-imidazo[4,5-b]pyridine;

- 2-ethyl-3-(1-ethyl-3-methoxypropyl)-7-(5-fluoro-4-methoxy-2-methylphenyl)-3H-imidazo[4,5-b]pyridine;
- 3-(1-ethyl-3-methoxypropyl)-7-(5-fluoro-4-methoxy-2-methylphenyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-5-fluoro-4-methylphenyl)-2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridine;
- 10 7-(2-chloro-5-fluoro-4-methylphenyl)-3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 7-[2-chloro-4-(methylsulfonyl)phenyl]-2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridine;
- 15 7-[2-chloro-4-(methylsulfonyl)phenyl]-3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 1-{3-chloro-4-[2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridin-7-yl]phenyl}-1-ethanone;
- 20 1-{3-chloro-4-[3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridin-7-yl]phenyl}-1-ethanone;
- 1-{5-[2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridin-7-yl]-6-methyl-2-pyridinyl}-1-ethanone;
- 1-{5-[3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridin-7-yl]-6-methyl-2-pyridinyl}-1-ethanone;
- 30 2-ethyl-3-(1-ethyl-3-methoxypropyl)-7-(6-methoxy-2-methyl-3-pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 3-(1-ethyl-3-methoxypropyl)-2-methoxy-7-(6-methoxy-2-methyl-3-pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 35 7-(2,6-dimethoxy-3-pyridinyl)-2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridine;

- 7-(2,6-dimethoxy-3-pyridinyl)-3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 5 7-(2,6-dimethyl-3-pyridinyl)-2-ethyl-3-(1-ethyl-3-methoxypropyl)-3H-imidazo[4,5-b]pyridine;
- 7-(2,6-dimethyl-3-pyridinyl)-3-(1-ethyl-3-methoxypropyl)-2-methoxy-3H-imidazo[4,5-b]pyridine;
- 10 2-ethyl-3-(1-ethyl-3-methoxypropyl)-7-(2,5,6-trimethyl-3-pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 3-(1-ethyl-3-methoxypropyl)-2-methoxy-7-(2,5,6-trimethyl-3-pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 15 7-(2,4-dichlorophenyl)-2-ethyl-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 20 7-(2,4-dichlorophenyl)-2-methoxy-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 7-[2-chloro-4-(trifluoromethyl)phenyl]-2-ethyl-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 25 7-[2-chloro-4-(trifluoromethyl)phenyl]-2-methoxy-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 7-(2-chloro-5-fluoro-4-methylphenyl)-2-ethyl-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 30 7-(2-chloro-5-fluoro-4-methylphenyl)-2-methoxy-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 35 2-ethyl-7-(4-methoxy-2,5-dimethylphenyl)-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;

- 2-methoxy-7-(4-methoxy-2,5-dimethylphenyl)-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 2-ethyl-7-(5-fluoro-4-methoxy-2-methylphenyl)-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 5 7-(5-fluoro-4-methoxy-2-methylphenyl)-2-methoxy-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 10 2-ethyl-3-[1-(methoxymethyl)propyl]-7-(6-methoxy-2-methyl-3-pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 2-methoxy-3-[1-(methoxymethyl)propyl]-7-(6-methoxy-2-methyl-3-pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 15 7-(2,6-dimethoxy-3-pyridinyl)-2-ethyl-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 7-(2,6-dimethoxy-3-pyridinyl)-2-methoxy-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 20 7-(2,6-dimethyl-3-pyridinyl)-2-ethyl-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 25 7-(2,6-dimethyl-3-pyridinyl)-2-methoxy-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;
- 2-ethyl-3-[1-(methoxymethyl)propyl]-7-(2,5,6-trimethyl-3-pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 30 2-methoxy-3-[1-(methoxymethyl)propyl]-7-(2,5,6-trimethyl-3-pyridinyl)-3H-imidazo[4,5-b]pyridine;
- 7-[2-chloro-4-(methylsulfonyl)phenyl]-2-ethyl-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine; and
- 35 7-[2-chloro-4-(methylsulfonyl)phenyl]-2-methoxy-3-[1-(methoxymethyl)propyl]-3H-imidazo[4,5-b]pyridine;

or a pharmaceutically acceptable salt form thereof.

[2j] In another more preferred embodiment, the present
5 invention provides a novel compound of formula Ia, wherein:

R¹ is C₃₋₈ cycloalkyl;

10 R¹ is substituted with 0-1 substituents selected from the
group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, -NR^{15a}COR^{13a},
-N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b},
-CONR^{13a}R^{16a}, 1-morpholinyl, 1-piperidinyl,
1-piperazinyl, and C₄₋₈ cycloalkyl, wherein 0-1 carbon
15 atoms in the C₄₋₈ cycloalkyl is replaced by a group
selected from the group -O-, -S(O)_n-, -NR^{13a}-,
-NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-, and wherein N₄ in
1-piperazinyl is substituted with 0-1 substituents
selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and
SO₂R^{14b}; and,

20 R¹ is also substituted with 0-3 substituents independently
selected at each occurrence from the group R^{1a}, R^{1b},
R^{1c}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F,
I, C₁₋₄ haloalkyl, -OR^{13a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and
25 -NR^{13a}R^{16a}.

[2k] In another even more preferred embodiment, the present
invention provides a novel compound of formula Ia, wherein:

30

X is selected from the group O, S(O)_n and a bond;

n is 0, 1 or 2;

35 R¹ is selected from the group cyclopropyl, cyclobutyl, and
cyclopentyl;

5 R^1 is substituted with 0-1 substituents selected from the group -CN, $-S(O)_nR^{14b}$, $-COR^{13a}$, $-CO_2R^{13a}$, and C_{4-8} cycloalkyl, wherein one carbon atom in the C_{4-8} cycloalkyl is replaced by a group selected from the group -O-, $-S(O)_n$ -, $-NR^{13a}$ -, $-NCO_2R^{14b}$ -, $-NCOR^{14b}$ - and $-NSO_2R^{14b}$ -;

10 R^1 is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a} , R^{1b} , C_{1-6} alkyl, C_{2-8} alkenyl, C_{2-8} alkynyl, Br, Cl, F, CF_3 , CF_2CF_3 , $-OR^{13a}$, C_{1-2} alkoxy- C_{1-2} alkyl, and $-NR^{13a}R^{16a}$;

15 R^{1a} is aryl and is selected from the group phenyl and indanyl, each R^{1a} being substituted with 0-1 $-OR^{17}$ and 0-5 substituents independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, C_{1-4} haloalkyl, -CN, $-S(O)_nR^{18}$, $-COR^{17}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$;

20 R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, furanyl, thienyl, imidazolyl, thiazolyl, pyrrolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-4 carbon atoms with a substituent
25 independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, CF_3 , -CN, $-OR^{17}$, $-S(O)_nR^{18}$, $-COR^{17}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group
30 R^{15a} , CO_2R^{14b} , COR^{14b} and SO_2R^{14b} ;

R^2 is selected from the group C_{1-4} alkyl, C_{2-4} alkenyl, and C_{2-4} alkynyl and is substituted with 0-1 substituents selected from the group -CN, OH, Cl, F, and C_{1-4}
35 alkoxy;

- R⁹ is independently selected at each occurrence from the group H, C₁₋₄ alkyl and C₃₋₈ cycloalkyl;
- 5 R³ and R⁸ are independently selected at each occurrence from the group H, Br, Cl, F, -CN, C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₁₋₄ alkoxy, NH₂, C₁₋₄ alkylamino, and (C₁₋₄ alkyl)₂-amino;
- 10 R¹³ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;
- 15 R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 20 R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;
- 25 R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;
- 30 R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;
- 35 R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, C₁₋₄ haloalkyl, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

- R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 5 R¹⁷, R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;
- 10 alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;
- 15 R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ haloalkyl;
- 20 aryl is phenyl substituted with 1-4 substituents independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, -OR¹⁷, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷, -CO₂R¹⁷, -NR¹⁵COR¹⁷, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹; and,
- 25 heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 1-4 carbon atoms with a substituent independently selected
- 35

- at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and
- 5 each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and SO₂R^{14a}.
- 10 [21] In another still more preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:
- X is selected from the group O, S and a bond;
- 15 R¹ is substituted with 0-1 substituents selected from the group -CN, -CO₂R^{13a}, and C₄₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;
- 20 R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃, CF₃, -OR^{13a}, -OH, -OCH₃, -OCH₂CH₃, -CH₂OCH₃, -
- 25 CH₂CH₂OCH₃, and -NR^{13a}R^{16a};
- R^{1a} is aryl and is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-3 substituents independently selected at
- 30 each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂;
- 35 R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each

- heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, cyclopropyl, OCH_3 , OCH_2CH_3 , $\text{OCH}(\text{CH}_3)_2$, $\text{OCH}_2\text{CH}_2\text{CH}_3$, OCF_3 , Br, Cl, F, CF_3 , -CN, SCH_3 , $-\text{NH}_2$, $-\text{NHCH}_3$, $-\text{N}(\text{CH}_3)_2$, $-\text{C}(\text{O})\text{NH}_2$, $-\text{C}(\text{O})\text{NHCH}_3$, and $-\text{C}(\text{O})\text{N}(\text{CH}_3)_2$ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH_3 , CO_2CH_3 , COCH_3 and SO_2CH_3 ;
- R^2 is selected from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, and $\text{CH}_2\text{CH}_2\text{CH}_3$;
- R^3 and R^8 are independently selected at each occurrence from the group H, CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, and $\text{CH}_2\text{CH}_2\text{CH}_3$;
- aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, cyclopropyl, OCH_3 , OCH_2CH_3 , $\text{OCH}(\text{CH}_3)_2$, $\text{OCH}_2\text{CH}_2\text{CH}_3$, OCF_3 , Br, Cl, F, CF_3 , -CN, SCH_3 , SO_2CH_3 , $-\text{NH}_2$, $-\text{NHCH}_3$, $-\text{N}(\text{CH}_3)_2$, $-\text{C}(\text{O})\text{NH}_2$, $-\text{C}(\text{O})\text{NHCH}_3$, and $-\text{C}(\text{O})\text{N}(\text{CH}_3)_2$; and,
- heteroaryl is independently selected at each occurrence from the group pyridyl, indolyl, benzothienyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indoliny, and benzoxazolin-2-on-yl, each heteroaryl being substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, cyclopropyl, OCH_3 , OCH_2CH_3 , $\text{OCH}(\text{CH}_3)_2$, $\text{OCH}_2\text{CH}_2\text{CH}_3$, OCF_3 , Br, Cl, F, CF_3 , -CN, SCH_3 , SO_2CH_3 , $-\text{NH}_2$, $-\text{NHCH}_3$, $-\text{N}(\text{CH}_3)_2$, $-\text{C}(\text{O})\text{NH}_2$, $-\text{C}(\text{O})\text{NHCH}_3$, and $-\text{C}(\text{O})\text{N}(\text{CH}_3)_2$ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH_3 , CO_2CH_3 , COCH_3 and SO_2CH_3 .

[2m] In another further preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

5

R^1 is substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a} , R^{1b} , CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $CH_2CH_2CH_3$, $-(CH_2)_3CH_3$, $-CH=CH_2$, $-CH=CH(CH_3)$, $-CH\equiv CH$, $-CH\equiv C(CH_3)$, $-CH_2OCH_3$, $-CH_2CH_2OCH_3$, F, and CF_3 ;

10

R^{1a} is phenyl substituted with 0-1 substituents selected from OCH_3 , OCH_2CH_3 , $OCH(CH_3)_2$, $OCH_2CH_2CH_3$, and OCF_3 , and 0-2 substituents independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $CH_2CH_2CH_3$, Br, Cl, F, CF_3 , $-CN$, and SCH_3 ;

15

R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, and tetrazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $CH_2CH_2CH_3$, OCH_3 , OCH_2CH_3 , OCF_3 , Br, Cl, F, CF_3 , $-CN$, and SCH_3 and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH_3 , CO_2CH_3 , $COCH_3$ and SO_2CH_3 ;

20

25

R^2 is selected from the group CH_3 , CH_2CH_3 , and $CH(CH_3)_2$;

30

R^3 and R^8 are independently selected at each occurrence from the group H and CH_3 ;

35

aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $CH_2CH_2CH_3$, cyclopropyl, OCH_3 , OCH_2CH_3 , $OCH(CH_3)_2$, $OCH_2CH_2CH_3$, OCF_3 , Br, Cl, F,

CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,
-C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

heteroaryl is pyridyl substituted on 2-4 carbon atoms with
5 a substituent independently selected at each
occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂,
CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂,
OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃,
-NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and
10 -C(O)N(CH₃)₂.

[2n] In another even further preferred embodiment, the present
invention provides a novel compound of formula Ia, wherein:

15 R¹ is substituted with 0-2 substituents independently
selected at each occurrence from the group R^{1a}, CH₃,
CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH₂OCH₃, -
CH₂CH₂OCH₃, F, and CF₃; and,

20 R^{1a} is phenyl substituted with 0-2 substituents
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃,
-CN, and SCH₃.

25 [2o] In a still further preferred embodiment, the present
invention provides a novel compound of formula Ia, wherein:

30 D is phenyl substituted with 2-4 substituents independently
selected at each occurrence from the group CH₃, CH₂CH₃,
CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃,
OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

35 [2p] In another still further preferred embodiment, the
present invention provides a novel compound of formula Ia,
wherein:

D is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃,
5 cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

[2q] In another more preferred embodiment, the present
10 invention provides a novel compound of formula Ia, wherein:

R¹ is selected from the group C₁₋₁₀ alkyl, C₂₋₁₀ alkenyl, C₂₋₁₀ alkynyl, C₃₋₈ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ alkoxy-C₁₋₄ alkyl;

15 R¹ is substituted with a C₃₋₈ cycloalkyl group, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl group is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-;

20 R¹ is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, R^{1c}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₈ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;

30 R^{1a} is aryl and is selected from the group phenyl, naphthyl, indanyl and indenyl, each R^{1a} being substituted with 0-1 -OR¹⁷ and 0-5 substituents independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro,
35 SH, -S(O)_nR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷,

-N(COR¹⁷)₂, -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a},
and -CONR^{17a}R^{19a};

- R^{1b} is heteroaryl and is selected from the group pyridyl,
 5 pyrimidinyl, triazinyl, furanyl, quinolinyl,
 isoquinolinyl, thienyl, imidazolyl, thiazolyl,
 indolyl, pyrrolyl, oxazolyl, benzofuranyl,
 benzothienyl, benzothiazolyl, benzoxazolyl,
 isoxazolyl, pyrazolyl, triazolyl, tetrazolyl,
 10 indazolyl, 2,3-dihydrobenzofuranyl,
 2,3-dihydrobenzothienyl,
 2,3-dihydrobenzothienyl-S-oxide,
 2,3-dihydrobenzothienyl-S-dioxide, indolinyl,
 benzoxazolin-2-onyl, benzodioxolanyl and benzodioxane,
 15 each heteroaryl being substituted on 0-4 carbon atoms
 with a substituent independently selected at each
 occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl,
 Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH,
 -S(O)_mR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂,
 20 -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and
 -CONR^{17a}R^{19a} and each heteroaryl being substituted on
 any nitrogen atom with 0-1 substituents selected from
 the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b}; and,
- 25 R^{1c} is heterocyclyl and is a saturated or partially
 saturated heteroaryl, each heterocyclyl being
 substituted on 0-4 carbon atoms with a substituent
 independently selected at each occurrence from the
 group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄
 30 haloalkyl, -CN, nitro, -OR^{13a}, SH, -S(O)_nR^{14b}, -COR^{13a},
 -OC(O)R^{14b}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a},
 -NR^{15a}CO₂R^{14b}, -NR^{13a}R^{16a}, and -CONR^{13a}R^{16a} and each
 heterocyclyl being substituted on any nitrogen atom
 with 0-1 substituents selected from the group R^{13a},
 35 CO₂R^{14b}, COR^{14b} and SO₂R^{14b} and wherein any sulfur atom
 is optionally monooxidized or dioxidized.

[2r] In another even more preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

5 X is selected from the group O, S(O)_n and a bond;

n is 0, 1 or 2;

10 R¹ is selected from the group C₁₋₆ alkyl, C₂₋₆ alkenyl, C₂₋₆ alkynyl, and C₃₋₈ cycloalkyl;

15 R¹ is substituted with a C₃₋₆ cycloalkyl group, wherein 0-1 carbon atoms in the C₄₋₆ cycloalkyl group is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;

20 R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃, CF₂CF₃, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

25 R^{1a} is aryl and is selected from the group phenyl and indanyl, each R^{1a} being substituted with 0-1 -OR¹⁷ and 0-5 substituents independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷,
30 -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a};

35 R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, furanyl, thienyl, imidazolyl, thiazolyl, pyrrolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the

- group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, CF₃, -CN, -OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a} and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};
- R² is selected from the group C₁₋₄ alkyl, C₂₋₄ alkenyl, and C₂₋₄ alkynyl and is substituted with 0-1 substituents selected from the group -CN, OH, Cl, F, and C₁₋₄ alkoxy;
- R⁹ is independently selected at each occurrence from the group H, C₁₋₄ alkyl and C₃₋₈ cycloalkyl;
- R³ and R⁸ are independently selected at each occurrence from the group H, Br, Cl, F, -CN, C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₁₋₄ alkoxy, NH₂, C₁₋₄ alkylamino, and (C₁₋₄ alkyl)₂-amino;
- R¹³ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;
- R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;
- R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;

- R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;
- 5 R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, C₁₋₄ haloalkyl, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and
10 dimethylamino;
- R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
15
- R¹⁷, R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;
20
- alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in
25 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;
- R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ haloalkyl;
30
- aryl is phenyl substituted with 1-4 substituents independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, -OR¹⁷, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷, -CO₂R¹⁷,
35 -NR¹⁵COR¹⁷, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹; and,

heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 1-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and SO₂R^{14a}.

20

[2s] In another still more preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

25 X is selected from the group O, S and a bond;

R¹ is C₁₋₆ alkyl;

30 R¹ is substituted with a C₃₋₆ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₆ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;

35 R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, F, CF₃, -OR^{13a}, -NR^{13a}R^{16a}, -CH₂OCH₃, -CH₂CH₂OCH₃, and C₃₋₆ cycloalkyl

which is substituted with 0-1 CH₃ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;

5

R^{1a} is aryl and is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-3 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂;

10

R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

20

25

R² is selected from the group CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

R³ and R⁸ are independently selected at each occurrence from the group H, CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

30

aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

35

heteroaryl is independently selected at each occurrence from the group pyridyl, indolyl, benzothienyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, and benzoxazolin-2-on-yl, each heteroaryl being substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃.

[2t] In another further preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:

R¹ is (cyclopropyl)C₁ alkyl or (cyclobutyl)C₁ alkyl;

R¹ is substituted with 1-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃, F, CF₃, cyclopropyl, CH₃-cyclopropyl, cyclobutyl, CH₃-cyclobutyl, cyclopentyl, CH₃-cyclopentyl;

R^{1a} is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, and OCF₃, and 0-2 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃, -CN, and SCH₃;

R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl,

- pyrazolyl, triazolyl, and tetrazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, and SCH₃ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;
- 10 R² is selected from the group CH₃, CH₂CH₃, and CH(CH₃)₂;
- R³ and R⁸ are independently selected at each occurrence from the group H and CH₃;
- 15 aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,
- 20 heteroaryl is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂.
- 25
- 30 [2u] In another even further preferred embodiment, the present invention provides a novel compound of formula Ia, wherein:
- R¹ is (cyclopropyl)C₁ alkyl or (cyclobutyl)C₁ alkyl;
- 35 R¹ is substituted with 1-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -

CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃,
F, CF₃, cyclopropyl, and CH₃-cyclopropyl;

R^{1a} is phenyl substituted with 0-2 substituents

5 independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃,
-CN, and SCH₃;

R^{1b} is heteroaryl and is selected from the group furanyl,

10 thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl,
and pyrazolyl, each heteroaryl being substituted on
0-3 carbon atoms with a substituent independently
selected at each occurrence from the group CH₃, CH₂CH₃,
CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F,
15 CF₃, -CN, and SCH₃.

[2v] In another further preferred embodiment, the present
invention provides a novel compound of formula Ia, wherein:

20

D is phenyl substituted with 2-4 substituents independently
selected at each occurrence from the group CH₃, CH₂CH₃,
CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃,
OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

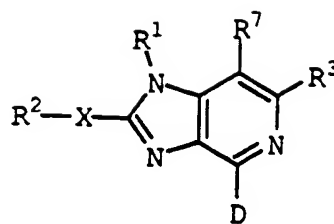
25

[2w] In another further preferred embodiment, the present
invention provides a novel compound of formula Ia, wherein:

30 D is pyridyl substituted on 2-4 carbon atoms with a
substituent independently selected at each occurrence
from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃,
cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃,
Br, Cl, F, and CF₃.

35

[3] In another preferred embodiment, the present invention
provides a novel compound of formula Ib:



(Ib).

5

[3a] In another more preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

X is selected from the group O, S(O)_n and a bond;

10

n is 0, 1 or 2;

R¹ is selected from the group C₁₋₆ alkyl, C₂₋₆ alkenyl, C₂₋₆ alkynyl, and C₃₋₈ cycloalkyl;

15

R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-;

20

R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃, CF₂CF₃, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₈ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

25

30

provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;

R^{1a} is aryl and is selected from the group phenyl and indanyl, each R^{1a} being substituted with 0-1 -OR¹⁷ and 0-5 substituents independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷,
5 -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a};

R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, furanyl, thienyl, imidazolyl, thiazolyl, pyrrolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, CF₃, -CN, -OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a}
10 and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

20 provided that R¹ is other than a -(CH₂)₁₋₄-aryl or -(CH₂)₁₋₄-heteroaryl wherein the aryl or heteroaryl group is substituted or unsubstituted;

R² is selected from the group C₁₋₄ alkyl, C₂₋₄ alkenyl, and C₂₋₄ alkynyl and is substituted with 0-1 substituents selected from the group -CN, OH, Cl, F, and C₁₋₄ alkoxy;

R³ and R⁷ are independently selected at each occurrence from the group H, Br, Cl, F, -CN, C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₁₋₄ alkoxy, NH₂, C₁₋₄ alkylamino, and (C₁₋₄ alkyl)₂-amino;

R⁹ is independently selected at each occurrence from the group H, C₁₋₄ alkyl and C₃₋₈ cycloalkyl;

- R¹³ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;
- 5 R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 10 R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;
- 15 R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;
- R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;
- 20 R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, C₁₋₄ haloalkyl, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;
- 25 R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 30 R¹⁷, R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;
- 35

alternatively, in an $\text{NR}^{17}\text{R}^{19}$ moiety, R^{17} and R^{19} taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N_4 in 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13} , CO_2R^{14} , COR^{14} and SO_2R^{14} ;

R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C_{1-6} alkyl, C_{3-10} cycloalkyl, C_{3-6} cycloalkyl- C_{1-6} alkyl and C_{1-4} haloalkyl;

aryl is phenyl substituted with 1-4 substituents independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, $-\text{OR}^{17}$, Br, Cl, F, C_{1-4} haloalkyl, $-\text{CN}$, $-\text{S}(\text{O})_n\text{R}^{18}$, $-\text{COR}^{17}$, $-\text{CO}_2\text{R}^{17}$, $-\text{NR}^{15}\text{COR}^{17}$, $-\text{NR}^{15}\text{CO}_2\text{R}^{18}$, $-\text{NR}^{17}\text{R}^{19}$, and $-\text{CONR}^{17}\text{R}^{19}$; and,

heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 1-4 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, C_{1-4} haloalkyl, $-\text{CN}$, $-\text{OR}^{17}$, $-\text{S}(\text{O})_m\text{R}^{18}$, $-\text{COR}^{17}$, $-\text{CO}_2\text{R}^{17}$, $-\text{OC}(\text{O})\text{R}^{18}$, $-\text{NR}^{15}\text{COR}^{17}$, $-\text{N}(\text{COR}^{17})_2$, $-\text{NR}^{15}\text{CO}_2\text{R}^{18}$, $-\text{NR}^{17}\text{R}^{19}$, and $-\text{CONR}^{17}\text{R}^{19}$ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15} , $\text{CO}_2\text{R}^{14a}$, COR^{14a} and $\text{SO}_2\text{R}^{14a}$.

[3b] In another even more preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

X is selected from the group O, S and a bond;

5

R¹ is substituted C₁₋₆ alkyl;

10 R¹ is substituted with 0-1 substituents selected from the group -CN, -CO₂R^{13a}, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;

15 R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl which is substituted with 0-1 CH₃ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by
20 -O-;

provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;

25 R^{1a} is aryl and is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-3 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and
30 -C(O)N(CH₃)₂;

35 R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂,

OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group
5 CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

provided that R¹ is other than a -(CH₂)₁₋₄-aryl or
-(CH₂)₁₋₄-heteroaryl wherein the aryl or heteroaryl
group is substituted or unsubstituted;

10

R² is selected from the group CH₃, CH₂CH₃, CH(CH₃)₂, and
CH₂CH₂CH₃;

R³ and R⁷ are independently selected at each occurrence from
15 the group H, CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

aryl is phenyl substituted with 2-4 substituents
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl,
20 OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F,
CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,
-C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

heteroaryl is independently selected at each occurrence from
25 the group pyridyl, indolyl, benzothienyl,
2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl,
2,3-dihydrobenzothienyl-S-oxide,
2,3-dihydrobenzothienyl-S-dioxide, indolinyl, and
benzoxazolin-2-on-yl, each heteroaryl being
30 substituted on 2-4 carbon atoms with a substituent
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl,
OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F,
CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,
35 -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each
heteroaryl being substituted on any nitrogen atom with
0-1 substituents selected from the group CH₃, CO₂CH₃,
COCH₃ and SO₂CH₃.

[3c] In another still more preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

5

R¹ is substituted C₁;

R¹ is substituted with 0-1 substituents selected from the group -CN, -CO₂CH₃, and -CO₂CH₂CH₃;

10

R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃, F, CF₃, cyclopropyl, CH₃-cyclopropyl, cyclobutyl, CH₃-cyclobutyl, cyclopentyl, CH₃-cyclopentyl;

15

R^{1a} is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, and OCF₃, and 0-2 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃, -CN, and SCH₃;

20

R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, and tetrazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, and SCH₃ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

25

30

provided that R¹ is other than a -(CH₂)₁₋₄-aryl or -(CH₂)₁₋₄-heteroaryl wherein the aryl or heteroaryl group is substituted or unsubstituted;

R² is selected from the group CH₃, CH₂CH₃, and CH(CH₃)₂;

R³ and R⁷ are independently selected at each occurrence from the group H and CH₃;

5

aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

10

20

heteroaryl is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂.

[3d] In another further preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

25 R¹ is substituted (cyclopropyl)-C₁ alkyl or (cyclobutyl)-C₁ alkyl;

R¹ is substituted with 0-1 -CN;

30 R¹ is also substituted with 0-1 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -CH=CH(CH₃), -CH=CH, -CH=C(CH₃), Br, Cl, F, CF₃, cyclopropyl, and CH₃-cyclopropyl;

35

R¹ is also substituted with 0-1 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -

CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃,
F, CF₃, cyclopropyl, and CH₃-cyclopropyl;

5 R^{1b} is heteroaryl and is selected from the group furanyl,
thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl,
and pyrazolyl, each heteroaryl being substituted on
0-3 carbon atoms with a substituent independently
selected at each occurrence from the group CH₃, CH₂CH₃,
CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F,
10 CF₃, -CN, and SCH₃.

[3e] In another further preferred embodiment, the present
invention provides a novel compound of formula Ib, wherein:

15 R¹ is (cyclopropyl)C₁ alkyl or (cyclobutyl)-C₁ alkyl
substituted with 1 substituent independently selected
at each occurrence from the group R^{1a}, R^{1b}, CH₃,
CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -
20 CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃,
F, CF₃, cyclopropyl, and CH₃-cyclopropyl;

R^{1a} is phenyl substituted with 0-2 substituents
independently selected at each occurrence from the
25 group CH₃, CH₂CH₃, Cl, F, and CF₃;

R^{1b} is heteroaryl and is selected from the group furanyl,
thienyl, and isoxazolyl, each heteroaryl being
substituted on 0-2 carbon atoms with a substituent
independently selected at each occurrence from the
30 group CH₃, OCH₃, Cl, F, and CF₃.

[3f] In an even further preferred embodiment, the present
35 invention provides a novel compound of formula Ib, wherein:

R¹ is selected from the group (cyclopropyl)CH-CH₃,
(cyclopropyl)CH-CH₂CH₃, (cyclopropyl)CH-CH₂OCH₃,

(cyclopropyl)CH-CH₂CH₂CH₃, (cyclopropyl)CH-CH₂CH₂OCH₃,
(cyclopropyl)₂CH, phenyl(cyclopropyl)CH,
furanyl(cyclopropyl)CH, thienyl(cyclopropyl)CH,
isoxazolyl(cyclopropyl)CH, (CH₃-
5 furanyl)(cyclopropyl)CH, (cyclobutyl)CH-CH₃,
(cyclobutyl)CH-CH₂CH₃, (cyclobutyl)CH-CH₂OCH₃,
(cyclobutyl)CH-CH₂CH₂CH₃, (cyclobutyl)CH-CH₂CH₂OCH₃,
(cyclobutyl)₂CH, phenyl(cyclobutyl)CH,
furanyl(cyclobutyl)CH, thienyl(cyclobutyl)CH,
10 isoxazolyl(cyclobutyl)CH, and (CH₃-
furanyl)(cyclobutyl)CH;

[3g] In another further preferred embodiment, the present
15 invention provides a novel compound of formula Ib, wherein:

D is phenyl substituted with 2-4 substituents independently
selected at each occurrence from the group CH₃, CH₂CH₃,
CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃,
20 OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

[3h] In another further preferred embodiment, the present
invention provides a novel compound of formula Ib, wherein:

25 D is pyridyl substituted on 2-4 carbon atoms with a
substituent independently selected at each occurrence
from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃,
cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃,
30 Br, Cl, F, and CF₃.

[3i] In another preferred embodiment, the present invention
provides a novel compound of formula Ib, wherein the compound
35 is selected from the group:

1-(1-cyclopropylpropyl)-4-(2,4-dichlorophenyl)-2-ethyl-1H-
imidazo[4,5-c]pyridine;

- 1-(1-cyclopropylpropyl)-4-(2,4-dichlorophenyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 5 1-(1-cyclopropylpropyl)-2-ethyl-4-[2-methyl-4-(trifluoromethyl)phenyl]-1H-imidazo[4,5-c]pyridine;
- 4-[2-chloro-4-(trifluoromethyl)phenyl]-1-(1-cyclopropylpropyl)-2-ethyl-1H-imidazo[4,5-c]pyridine;
- 10 4-[2-chloro-4-(trifluoromethyl)phenyl]-1-(1-cyclopropylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 4-[2-chloro-4-(trifluoromethyl)phenyl]-1-(1-cyclopropylpropyl)-2-(methylsulfanyl)-1H-imidazo[4,5-c]pyridine;
- 15 4-(2-chloro-4-methoxyphenyl)-1-(1-cyclopropylpropyl)-2-ethyl-1H-imidazo[4,5-c]pyridine;
- 20 4-(2-chloro-4-methoxyphenyl)-1-(1-cyclopropylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 1-(1-cyclopropylpropyl)-2-ethyl-4-(4-methoxy-2,5-dimethylphenyl)-1H-imidazo[4,5-c]pyridine;
- 25 1-(1-cyclopropylpropyl)-2-methoxy-4-(4-methoxy-2,5-dimethylphenyl)-1H-imidazo[4,5-c]pyridine;
- 30 4-(2-chloro-4-methoxyphenyl)-1-(1-cyclopropylpropyl)-2-ethyl-1H-imidazo[4,5-c]pyridine;
- 4-(2-chloro-4-methoxyphenyl)-1-(1-cyclopropylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 35 4-(2-chloro-5-fluoro-4-methoxyphenyl)-1-(1-cyclopropylpropyl)-2-ethyl-1H-imidazo[4,5-c]pyridine;

- 4-(2-chloro-fluoro-4-methoxyphenyl)-1-(1-cyclopropylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 4-(2-chloro-5-fluoro-4-methylphenyl)-1-(1-cyclopropylpropyl)-
5 2-ethyl-1H-imidazo[4,5-c]pyridine;
- 2.4-(2-chloro-fluoro-4-methylphenyl)-1-(1-cyclopropylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 10 1-(1-cyclopropylpropyl)-2-methoxy-4-(2,4,5-trimethylphenyl)-1H-imidazo[4,5-c]pyridine;
- 1-(1-cyclopropylpropyl)-2-ethyl-4-(2,4,5-trimethylphenyl)-1H-imidazo[4,5-c]pyridine;
- 15 1-(1-cyclopropylpropyl)-2-ethyl-4-(2,5,6-trimethyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine
- 1-(1-cyclopropylpropyl)-2-methoxy-4-(2,5,6-trimethyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine;
- 20 1-(1-cyclopropylpropyl)-4-(2,6-dimethyl-3-pyridinyl)-2-ethyl-1H-imidazo[4,5-c]pyridine;
- 1-(1-cyclopropylpropyl)-4-(2,6-dimethyl-3-pyridinyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 25 1-(1-cyclopropylpropyl)-4-(2,6-dimethoxy-3-pyridinyl)-2-ethyl-1H-imidazo[4,5-c]pyridine;
- 30 4-(2,4-dichlorophenyl)-2-ethyl-1-(1-ethylpropyl)-1H-imidazo[4,5-c]pyridine;
- 4-(2,4-dichlorophenyl)-1-(1-ethylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 35 4-[2-chloro-4-(trifluoromethyl)phenyl]-1-(1-ethylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;

- 4-[2-chloro-4-(trifluoromethyl)phenyl]-2-ethyl-1-(1-ethylpropyl)-1H-imidazo[4,5-c]pyridine;
- 5 4-[2-chloro-4-(methylsulfonyl)phenyl]-2-ethyl-1-(1-ethylpropyl)-1H-imidazo[4,5-c]pyridine;
- 4-[2-chloro-4-(methylsulfonyl)phenyl]-1-(1-ethylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 10 2-ethyl-1-(1-ethylpropyl)-4-(4-methoxy-2,5-dimethylphenyl)-1H-imidazo[4,5-c]pyridine;
- 1- (1-ethylpropyl)-2-methoxy-4-(4-methoxy-2,5-dimethylphenyl)-1H-imidazo[4,5-c]pyridine;
- 15 4-(2-chloro-4-methoxyphenyl)-2-ethyl-1-(1-ethylpropyl)-1H-imidazo[4,5-c]pyridine;
- 20 4-(2-chloro-4-methoxyphenyl)-1-(1-ethylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 2-ethyl-1-(1-ethylpropyl)-4-[4-methoxy-2-(trifluoromethyl)phenyl]-1H-imidazo[4,5-c]pyridine;
- 25 1-(1-ethylpropyl)-2-methoxy-4-[4-methoxy-2-(trifluoromethyl)phenyl]-1H-imidazo[4,5-c]pyridine;
- 1-(1-ethylpropyl)-4-(5-fluoro-4-methoxy-2-methylphenyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 30 2-ethyl-1-(1-ethylpropyl)-4-(5-fluoro-4-methoxy-2-methylphenyl)-1H-imidazo[4,5-c]pyridine;
- 35 3-chloro-4-[1-(1-ethylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridin-4-yl]benzonitrile;

- 3-chloro-4-[2-ethyl-1-(1-ethylpropyl)-1H-imidazo[4,5-c]pyridin-4-yl]benzonitrile;
- 1-{3-chloro-4-[2-ethyl-1-(1-ethylpropyl)-1H-imidazo[4,5-c]pyridin-4-yl]phenyl}-1-ethanone;
- 1-{3-chloro-4-[1-(1-ethylpropyl)-2-methoxy-1H-imidazo[4,5-c]pyridin-4-yl]phenyl}-1-ethanone;
- 10 1-(dicyclopropylmethyl)-2-ethyl-4-(5-fluoro-4-methoxy-2-methylphenyl)-1H-imidazo[4,5-c]pyridine;
- 1-(dicyclopropylmethyl)-4-(5-fluoro-4-methoxy-2-methylphenyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 15 4-(2-chloro-4-methoxyphenyl)-1-(dicyclopropylmethyl)-2-ethyl-1H-imidazo[4,5-c]pyridine;
- 4-(2-chloro-4-methoxyphenyl)-1-(dicyclopropylmethyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 20 4-(2,4-dichlorophenyl)-1-(dicyclopropylmethyl)-2-ethyl-1H-imidazo[4,5-c]pyridine;
- 25 4-(2,4-dichlorophenyl)-1-(dicyclopropylmethyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 4-[2-chloro-4-(trifluoromethyl)phenyl]-1-(dicyclopropylmethyl)-2-ethyl-1H-imidazo[4,5-c]pyridine;
- 30 4-[2-chloro-4-(trifluoromethyl)phenyl]-1-(dicyclopropylmethyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 4-(2,4-dichlorophenyl)-1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 35 4-(2,4-dichlorophenyl)-2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridine;

- 4-[2-chloro-4-(trifluoromethyl)phenyl]-1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 5 4-[2-chloro-4-(trifluoromethyl)phenyl]-2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridine;
- 4-(2-chloro-4-methoxyphenyl)-1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 10 4-(2-chloro-4-methoxyphenyl)-2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridine;
- 4-(2-chloro-5-fluoro-4-methoxyphenyl)-1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 15 4-(2-chloro-5-fluoro-4-methoxyphenyl)-2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridine;
- 20 1-(1-ethyl-3-methoxypropyl)-2-methoxy-4-(4-methoxy-2,5-dimethylphenyl)-1H-imidazo[4,5-c]pyridine;
- 2-ethyl-1-(1-ethyl-3-methoxypropyl)-4-(4-methoxy-2,5-dimethylphenyl)-1H-imidazo[4,5-c]pyridine;
- 25 2-ethyl-1-(1-ethyl-3-methoxypropyl)-4-(5-fluoro-4-methoxy-2-methylphenyl)-1H-imidazo[4,5-c]pyridine;
- 1-(1-ethyl-3-methoxypropyl)-4-(5-fluoro-4-methoxy-2-methylphenyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 30 4-(2-chloro-5-fluoro-4-methylphenyl)-1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 35 4-(2-chloro-5-fluoro-4-methylphenyl)-2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridine;

- 4-[2-chloro-4-(methylsulfonyl)phenyl]-1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 5 4-[2-chloro-4-(methylsulfonyl)phenyl]-2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridine;
- 1-{3-chloro-4-[1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridin-4-yl]phenyl}-1-ethanone;
- 10 1-{3-chloro-4-[2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridin-4-yl]phenyl}-1-ethanone;
- 1-{5-[1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridin-4-yl]-6-methyl-2-pyridinyl}-1-ethanone;
- 15 1-{5-[2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridin-4-yl]-6-methyl-2-pyridinyl}-1-ethanone;
- 1-(1-ethyl-3-methoxypropyl)-2-methoxy-4-(6-methoxy-2-methyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine;
- 20 2-ethyl-1-(1-ethyl-3-methoxypropyl)-4-(6-methoxy-2-methyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine;
- 25 4-(2,6-dimethoxy-3-pyridinyl)-2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridine;
- 4-(2,6-dimethoxy-3-pyridinyl)-1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 30 4-(2,6-dimethyl-3-pyridinyl)-1-(1-ethyl-3-methoxypropyl)-2-methoxy-1H-imidazo[4,5-c]pyridine;
- 4-(2,6-dimethyl-3-pyridinyl)-2-ethyl-1-(1-ethyl-3-methoxypropyl)-1H-imidazo[4,5-c]pyridine;
- 35 2-ethyl-1-(1-ethyl-3-methoxypropyl)-4-(2,5,6-trimethyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine;

- 1-(1-ethyl-3-methoxypropyl)-2-methoxy-4-(2,5,6-trimethyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine;
- 5 4-(2,4-dichlorophenyl)-2-ethyl-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 4-(2,4-dichlorophenyl)-2-methoxy-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 10 4-[2-chloro-4-(trifluoromethyl)phenyl]-2-ethyl-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 4-[2-chloro-4-(trifluoromethyl)phenyl]-2-methoxy-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 15 4-(2-chloro-5-fluoro-4-methylphenyl)-2-ethyl-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 4-(2-chloro-5-fluoro-4-methylphenyl)-2-methoxy-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 20 2-methoxy-4-(4-methoxy-2,5-dimethylphenyl)-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 25 2-ethyl-4-(4-methoxy-2,5-dimethylphenyl)-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 2-ethyl-4-(5-fluoro-4-methoxy-2-methylphenyl)-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 30 4-(5-fluoro-4-methoxy-2-methylphenyl)-2-methoxy-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 35 2-methoxy-1-[1-(methoxymethyl)propyl]-4-(6-methoxy-2-methyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine;

- 2-ethyl-1-[1-(methoxymethyl)propyl]-4-(6-methoxy-2-methyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine;
- 4-(2,6-dimethoxy-3-pyridinyl)-2-ethyl-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 4-(2,6-dimethoxy-3-pyridinyl)-2-methoxy-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 4-(2,6-dimethyl-3-pyridinyl)-2-ethyl-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 4-(2,6-dimethyl-3-pyridinyl)-2-methoxy-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- 2-ethyl-1-[1-(methoxymethyl)propyl]-4-(2,5,6-trimethyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine;
- 2-methoxy-1-[1-(methoxymethyl)propyl]-4-(2,5,6-trimethyl-3-pyridinyl)-1H-imidazo[4,5-c]pyridine;
- 4-[2-chloro-4-(methylsulfonyl)phenyl]-2-ethyl-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine; and
- 4-[2-chloro-4-(methylsulfonyl)phenyl]-2-methoxy-1-[1-(methoxymethyl)propyl]-1H-imidazo[4,5-c]pyridine;
- or a pharmaceutically acceptable salt form thereof.

30

[3j] In another more preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

R¹ is C₃₋₈ cycloalkyl;

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R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b},

- CONR^{13a}R^{16a}, 1-morpholinyl, 1-piperidinyl, 1-piperazinyl, and C₄₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-,
 5 -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-, and wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b}; and,
- 10 R¹ is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, R^{1c}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -OR^{13a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and -NR^{13a}R^{16a}.
- 15
- [3k] In another even more preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:
- 20 X is selected from the group O, S(O)_n and a bond;
- n is 0, 1 or 2;
- R¹ is selected from the group cyclopropyl, cyclobutyl, and
 25 cyclopentyl;
- R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, and C₄₋₈ cycloalkyl, wherein one carbon atom in the C₄₋₈
 30 cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-;
- R¹ is also substituted with 0-2 substituents independently
 35 selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃, CF₂CF₃, -OR^{13a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and -NR^{13a}R^{16a};

- 5 R^{1a} is aryl and is selected from the group phenyl and indanyl, each R^{1a} being substituted with 0-1 $-OR^{17}$ and 0-5 substituents independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, C_{1-4} haloalkyl, $-CN$, $-S(O)_nR^{18}$, $-COR^{17}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$;
- 10 R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, furanyl, thienyl, imidazolyl, thiazolyl, pyrrolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, CF_3 , $-CN$, $-OR^{17}$, $-S(O)_mR^{18}$, $-COR^{17}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15a} , CO_2R^{14b} , COR^{14b} and SO_2R^{14b} ;
- 20 R^2 is selected from the group C_{1-4} alkyl, C_{2-4} alkenyl, and C_{2-4} alkynyl and is substituted with 0-1 substituents selected from the group $-CN$, OH, Cl, F, and C_{1-4} alkoxy;
- 25 R^9 is independently selected at each occurrence from the group H, C_{1-4} alkyl and C_{3-8} cycloalkyl;
- 30 R^3 and R^7 are independently selected at each occurrence from the group H, Br, Cl, F, $-CN$, C_{1-4} alkyl, C_{3-6} cycloalkyl, C_{1-4} alkoxy, NH_2 , C_{1-4} alkylamino, and $(C_{1-4} alkyl)_2$ -amino;
- 35 R^{13} is selected from the group C_{1-4} alkyl, C_{1-2} haloalkyl, C_{1-2} alkoxy- C_{1-2} alkyl, C_{3-6} cycloalkyl- C_{1-2} alkyl, aryl(C_{1-2} alkyl)-, and heteroaryl(C_{1-2} alkyl)-;

- R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 5 R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;
- 10 R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;
- R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;
- 15
- R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, C₁₋₄ haloalkyl, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;
- 20
- 25 R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- R¹⁷, R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;
- 30
- alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in
- 35

1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13} , CO_2R^{14} , COR^{14} and SO_2R^{14} ;

5 R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C_{1-6} alkyl, C_{3-10} cycloalkyl, C_{3-6} cycloalkyl- C_{1-6} alkyl and C_{1-4} haloalkyl;

10 aryl is phenyl substituted with 1-4 substituents independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, $-OR^{17}$, Br, Cl, F, C_{1-4} haloalkyl, $-CN$, $-S(O)_mR^{18}$, $-COR^{17}$, $-CO_2R^{17}$, $-NR^{15}COR^{17}$, $-NR^{15}CO_2R^{18}$, $-NR^{17}R^{19}$, and $-CONR^{17}R^{19}$; and,

15 heteroaryl is independently selected at each occurrence from: the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, tetrazolyl, indazolyl,
20 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 1-4
25 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, C_{1-4} haloalkyl, $-CN$, $-OR^{17}$, $-S(O)_mR^{18}$, $-COR^{17}$, $-CO_2R^{17}$, $-OC(O)R^{18}$, $-NR^{15}COR^{17}$, $-N(COR^{17})_2$, $-NR^{15}CO_2R^{18}$, $-NR^{17}R^{19}$, and $-CONR^{17}R^{19}$ and
30 each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15} , CO_2R^{14a} , COR^{14a} and SO_2R^{14a} .

35 [31] In another still more preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

X is selected from the group O, S and a bond;

5 R^1 is substituted with 0-1 substituents selected from the group -CN, $-\text{CO}_2R^{13a}$, and C_{4-8} cycloalkyl, wherein 0-1 carbon atoms in the C_{4-8} cycloalkyl is replaced by a group selected from the group -O-, $-\text{S}(\text{O})_n-$, and $-\text{NR}^{13a}-$;

10 R^1 is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a} , R^{1b} , C_{1-6} alkyl, C_{2-8} alkenyl, C_{2-8} alkynyl, Br, Cl, F, CF_3 , CF_3 , $-\text{OR}^{13a}$, -OH, -OCH₃, -OCH₂CH₃, -CH₂OCH₃, -CH₂CH₂OCH₃, and $-\text{NR}^{13a}R^{16a}$;

15 R^{1a} is aryl and is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-3 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, Br, Cl, F, CF_3 , -CN, SCH₃,
20 -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂;

R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl,
25 pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂,
30 OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF_3 , -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

35 R^2 is selected from the group CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

R³ and R⁷ are independently selected at each occurrence from the group H, CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

aryl is phenyl substituted with 2-4 substituents

5 independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

10

heteroaryl is independently selected at each occurrence from the group pyridyl, indolyl, benzothienyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide,

15

2,3-dihydrobenzothienyl-S-dioxide, indolinyl, and benzoxazolin-2-on-yl, each heteroaryl being

substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl,

20

OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each

heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃,

25

COCH₃ and SO₂CH₃.

[3m] In another further preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

30

R¹ is substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃, F, and CF₃;

35

R^{1a} is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and

0-2 substituents independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, Br, Cl, F, CF_3 , -CN, and SCH_3 ;

5 R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, and tetrazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a
10 substituent independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, OCH_3 , OCH_2CH_3 , OCF_3 , Br, Cl, F, CF_3 , -CN, and SCH_3 and each heteroaryl being substituted on any nitrogen atom with
15 0-1 substituents selected from the group CH_3 , CO_2CH_3 , COCH_3 and SO_2CH_3 ;

R^2 is selected from the group CH_3 , CH_2CH_3 , and $\text{CH}(\text{CH}_3)_2$;

R^3 and R^7 are independently selected at each occurrence from the group H and CH_3 ;

20 aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, cyclopropyl, OCH_3 , OCH_2CH_3 , $\text{OCH}(\text{CH}_3)_2$, $\text{OCH}_2\text{CH}_2\text{CH}_3$, OCF_3 , Br, Cl, F, CF_3 , -CN, SCH_3 , SO_2CH_3 , $-\text{NH}_2$, $-\text{NHCH}_3$, $-\text{N}(\text{CH}_3)_2$,
25 $-\text{C}(\text{O})\text{NH}_2$, $-\text{C}(\text{O})\text{NHCH}_3$, and $-\text{C}(\text{O})\text{N}(\text{CH}_3)_2$; and,

heteroaryl is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each
30 occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, cyclopropyl, OCH_3 , OCH_2CH_3 , $\text{OCH}(\text{CH}_3)_2$, $\text{OCH}_2\text{CH}_2\text{CH}_3$, OCF_3 , Br, Cl, F, CF_3 , -CN, SCH_3 , SO_2CH_3 , $-\text{NH}_2$, $-\text{NHCH}_3$, $-\text{N}(\text{CH}_3)_2$, $-\text{C}(\text{O})\text{NH}_2$, $-\text{C}(\text{O})\text{NHCH}_3$, and
35 $-\text{C}(\text{O})\text{N}(\text{CH}_3)_2$.

[3n] In another even further preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

R¹ is substituted with 0-2 substituents independently
selected at each occurrence from the group R^{1a}, CH₃,
CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH₂OCH₃, -
5 CH₂CH₂OCH₃, F, and CF₃; and,

R^{1a} is phenyl substituted with 0-2 substituents
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃,
10 -CN, and SCH₃.

[3o] In another still further preferred embodiment, the
present invention provides a novel compound of formula Ib,
15 wherein:

D is phenyl substituted with 2-4 substituents independently
selected at each occurrence from the group CH₃, CH₂CH₃,
CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃,
20 OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

[3p] In another still further preferred embodiment, the
present invention provides a novel compound of formula Ib,
25 wherein:

D is pyridyl substituted on 2-4 carbon atoms with a
substituent independently selected at each occurrence
from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃,
30 cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃,
Br, Cl, F, and CF₃.

[3q] In another more preferred embodiment, the present
35 invention provides a novel compound of formula Ib, wherein:

- R^1 is selected from the group C_{1-10} alkyl, C_{2-10} alkenyl, C_{2-10} alkynyl, C_{3-8} cycloalkyl, C_{3-6} cycloalkyl- C_{1-6} alkyl and C_{1-4} alkoxy- C_{1-4} alkyl;
- 5 R^1 is substituted with a C_{3-8} cycloalkyl group, wherein 0-1 carbon atoms in the C_{4-8} cycloalkyl group is replaced by a group selected from the group -O-, $-S(O)_n-$, $-NR^{13a}-$, $-NCO_2R^{14b}-$, $-NCOR^{14b}-$ and $-NSO_2R^{14b}-$;
- 10 R^1 is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a} , R^{1b} , R^{1c} , C_{1-6} alkyl, C_{2-8} alkenyl, C_{2-8} alkynyl, Br, Cl, F, I, C_{1-4} haloalkyl, $-OR^{13a}$, $-NR^{13a}R^{16a}$, C_{1-2} alkoxy- C_{1-2} alkyl, and C_{3-8} cycloalkyl which is substituted with 0-1 R^9 and in which 0-1 carbons of C_{4-8} cycloalkyl is
- 15 replaced by -O-;
- provided that R^1 is other than a cyclohexyl- $(CH_2)_2-$ group;
- 20 R^{1a} is aryl and is selected from the group phenyl, naphthyl, indanyl and indenyl, each R^{1a} being substituted with 0-1 $-OR^{17}$ and 0-5 substituents independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, -CN, nitro,
- 25 SH, $-S(O)_nR^{18}$, $-COR^{17}$, $-OC(O)R^{18}$, $-NR^{15a}COR^{17}$, $-N(COR^{17})_2$, $-NR^{15a}CONR^{17a}R^{19a}$, $-NR^{15a}CO_2R^{18}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$;
- R^{1b} is heteroaryl and is selected from the group pyridyl,
- 30 pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl,
- 35 indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide,

2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-onyl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH, -S(O)_mR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂, -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a} and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b}; and,

R^{1c} is heterocyclyl and is a saturated or partially saturated heteroaryl, each heterocyclyl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR^{13a}, SH, -S(O)_nR^{14b}, -COR^{13a}, -OC(O)R^{14b}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b}, -NR^{13a}R^{16a}, and -CONR^{13a}R^{16a} and each heterocyclyl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b} and wherein any sulfur atom is optionally monooxidized or dioxidized.

25

[3r] In another even more preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

30 X is selected from the group O, S(O)_n and a bond;

n is 0, 1 or 2;

35 R¹ is selected from the group C₁₋₆ alkyl, C₂₋₆ alkenyl, C₂₋₆ alkynyl, C₃₋₈ cycloalkyl;

R¹ is substituted with a C₃₋₆ cycloalkyl group, wherein 0-1 carbon atoms in the C₄₋₆ cycloalkyl group is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;

5

R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃, CF₂CF₃, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

10

R^{1a} is aryl and is selected from the group phenyl and indanyl, each R^{1a} being substituted with 0-1 -OR¹⁷ and 0-5 substituents independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a};

15

20

R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, furanyl, thienyl, imidazolyl, thiazolyl, pyrrolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, CF₃, -CN, -OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a} and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

25

30

R² is selected from the group C₁₋₄ alkyl, C₂₋₄ alkenyl, and C₂₋₄ alkynyl and is substituted with 0-1 substituents selected from the group -CN, OH, Cl, F, and C₁₋₄ alkoxy;

35

R⁹ is independently selected at each occurrence from the group H, C₁₋₄ alkyl and C₃₋₈ cycloalkyl;

5 R³ and R⁷ are independently selected at each occurrence from the group H, Br, Cl, F, -CN, C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₁₋₄ alkoxy, NH₂, C₁₋₄ alkylamino, and (C₁₋₄ alkyl)₂-amino;

10 R¹³ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;

15 R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

20 R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;

R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;

25 R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;

30 R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, C₁₋₄ haloalkyl, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and
35 dimethylamino;

- R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 5 R¹⁷, R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;
- 10 alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;
- 15 R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ haloalkyl;
- 20 aryl is phenyl substituted with 1-4 substituents independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, -OR¹⁷, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷, -CO₂R¹⁷, -NR¹⁵COR¹⁷, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹; and,
- 25 heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, 30 benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 1-4 carbon atoms with a substituent independently selected
- 35

- at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and
- 5 each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and SO₂R^{14a}.
- 10 [3s] In another still more preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:
- X is selected from the group O, S and a bond;
- 15 R¹ is C₁₋₆ alkyl;
- R¹ is substituted with a C₃₋₆ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₄ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;
- 20 R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, F, CF₃, -OR^{13a}, -NR^{13a}R^{16a}, -CH₂OCH₃, -CH₂CH₂OCH₃, and C₃₋₆ cycloalkyl
- 25 which is substituted with 0-1 CH₃ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;
- provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;
- 30 R^{1a} is aryl and is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-3 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, Br, Cl, F, CF₃, -CN, SCH₃,
- 35 -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂;

- R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;
- R² is selected from the group CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;
- R³ and R⁷ are independently selected at each occurrence from the group H, CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;
- aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,
- heteroaryl is independently selected at each occurrence from the group pyridyl, indolyl, benzothienyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, and benzoxazolin-2-on-yl, each heteroaryl being substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each

heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH_3 , CO_2CH_3 , COCH_3 and SO_2CH_3 .

5

[3t] In another further preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

R^1 is (cyclopropyl) C_1 alkyl or (cyclobutyl) C_1 alkyl;

10

R^1 is substituted with 1-2 substituents independently selected at each occurrence from the group R^{1a} , R^{1b} , CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, $-(\text{CH}_2)_3\text{CH}_3$, $-\text{CH}=\text{CH}_2$, $-\text{CH}=\text{CH}(\text{CH}_3)$, $-\text{CH}\equiv\text{CH}$, $-\text{CH}\equiv\text{C}(\text{CH}_3)$, $-\text{CH}_2\text{OCH}_3$, $-\text{CH}_2\text{CH}_2\text{OCH}_3$,
15 F, CF_3 , cyclopropyl, CH_3 -cyclopropyl, cyclobutyl, CH_3 -cyclobutyl, cyclopentyl, CH_3 -cyclopentyl;

20

R^{1a} is phenyl substituted with 0-1 substituents selected from OCH_3 , OCH_2CH_3 , and OCF_3 , and 0-2 substituents independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, Br, Cl, F, CF_3 , $-\text{CN}$, and SCH_3 ;

25

R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, and tetrazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, OCH_3 ,
30 OCH_2CH_3 , OCF_3 , Br, Cl, F, CF_3 , $-\text{CN}$, and SCH_3 and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH_3 , CO_2CH_3 , COCH_3 and SO_2CH_3 ;

35 R^2 is selected from the group CH_3 , CH_2CH_3 , and $\text{CH}(\text{CH}_3)_2$;

R^3 and R^7 are independently selected at each occurrence from the group H and CH_3 ;

aryl is phenyl substituted with 2-4 substituents
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl,
5 OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F,
CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,
-C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

heteroaryl is pyridyl substituted on 2-4 carbon atoms with
10 a substituent independently selected at each
occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂,
CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂,
OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃,
-NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and
15 -C(O)N(CH₃)₂.

[3u] In another even further preferred embodiment, the present
invention provides a novel compound of formula Ib, wherein:

20 R¹ is (cyclopropyl)C₁ alkyl or (cyclobutyl)C₁ alkyl;

R¹ is substituted with 1-2 substituents independently
selected at each occurrence from the group R^{1a}, R^{1b},
25 CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -
CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃,
F, CF₃, cyclopropyl, and CH₃-cyclopropyl;

R^{1a} is phenyl substituted with 0-2 substituents
30 independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃,
-CN, and SCH₃;

R^{1b} is heteroaryl and is selected from the group furanyl,
35 thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl,
and pyrazolyl, each heteroaryl being substituted on
0-3 carbon atoms with a substituent independently
selected at each occurrence from the group CH₃, CH₂CH₃,

CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, and SCH₃.

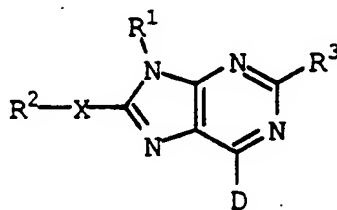
5 [3v] In another further preferred embodiment, the present invention provides a novel compound of formula Ib, wherein:

D is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃,
 10 CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

[3w] In another further preferred embodiment, the present
 15 invention provides a novel compound of formula Ib, wherein:

D is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃,
 20 cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

[4] In another preferred embodiment, the present invention
 25 provides a novel compound of formula Ic:



(Ic).

30

[4a] In another more preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

X is selected from the group O, S(O)_n and a bond;

n is 0, 1 or 2;

5 R^1 is selected from the group C_{1-6} alkyl, C_{2-6} alkenyl, C_{2-6} alkynyl, and C_{3-8} cycloalkyl;

10 R^1 is substituted with 0-1 substituents selected from the group $-CN$, $-S(O)_nR^{14b}$, $-COR^{13a}$, $-CO_2R^{13a}$, and C_{3-8} cycloalkyl, wherein 0-1 carbon atoms in the C_{4-8} cycloalkyl is replaced by a group selected from the group $-O-$, $-S(O)_n-$, $-NR^{13a}-$, $-NCO_2R^{14b}-$, $-NCOR^{14b}-$ and $-NSO_2R^{14b}-$;

15 R^1 is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a} , R^{1b} , C_{1-6} alkyl, C_{2-8} alkenyl, C_{2-8} alkynyl, Br, Cl, F, CF_3 , CF_2CF_3 , $-OR^{13a}$, $-NR^{13a}R^{16a}$, C_{1-2} alkoxy- C_{1-2} alkyl, and C_{3-8} cycloalkyl which is substituted with 0-1 R^9 and in which 0-1 carbons of C_{4-8} cycloalkyl is replaced by
20 $-O-$;

provided that R^1 is other than a cyclohexyl- $(CH_2)_2-$ group;

25 R^{1a} is aryl and is selected from the group phenyl and indanyl, each R^{1a} being substituted with 0-1 $-OR^{17}$ and 0-5 substituents independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, C_{1-4} haloalkyl, $-CN$, $-S(O)_nR^{18}$, $-COR^{17}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$;

30 R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, furanyl, thienyl, imidazolyl, thiazolyl, pyrrolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being
35 substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, CF_3 , $-CN$,

-OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a}
and each heteroaryl being substituted on any nitrogen
atom with 0-1 substituents selected from the group
R^{15a}, .CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

5

provided that R¹ is other than a -(CH₂)₁₋₄-aryl or
-(CH₂)₁₋₄-heteroaryl wherein the aryl or heteroaryl
group is substituted or unsubstituted;

10 R² is selected from the group C₁₋₄ alkyl, C₂₋₄ alkenyl, and
C₂₋₄ alkynyl and is substituted with 0-1 substituents
selected from the group -CN, OH, Cl, F, and C₁₋₄
alkoxy;

15 R³ is selected from the group H, Br, Cl, F, -CN, C₁₋₄ alkyl,
C₃₋₆ cycloalkyl, C₁₋₄ alkoxy, NH₂, C₁₋₄ alkylamino, and
(C₁₋₄ alkyl)₂-amino;

20 R⁹ is independently selected at each occurrence from the
group H, C₁₋₄ alkyl and C₃₋₈ cycloalkyl;

R¹³ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl,
C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl,
aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;

25

R^{13a} and R^{16a} are independently selected at each occurrence
from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄
alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-
C₁₋₆ alkyl;

30

R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl,
C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl,
aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;

35 R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl,
C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;

R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;

5 R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, C₁₋₄
10 haloalkyl, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆
15 cycloalkyl-C₁₋₆ alkyl;

R¹⁷, R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂
20 alkyl, and C₁₋₄ haloalkyl;

alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in
25 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;

R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆
30 cycloalkyl-C₁₋₆ alkyl and C₁₋₄ haloalkyl;

aryl is phenyl substituted with 1-4 substituents independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, -OR¹⁷, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷, -CO₂R¹⁷,
35 -NR¹⁵COR¹⁷, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹; and,

heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 1-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -OR¹⁷, -S(O)_nR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and SO₂R^{14a}.

20

[4b] In another even more preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

25 X is selected from the group O, S and a bond;

R¹ is substituted C₁₋₆ alkyl;

30 R¹ is substituted with 0-1 substituents selected from the group -CN, -CO₂R^{13a}, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;

35 R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃,

-OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl which is substituted with 0-1 CH₃ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

5

provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;

R^{1a} is aryl and is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-3 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂;

15

R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

20

25

provided that R¹ is other than a -(CH₂)₁₋₄-aryl or -(CH₂)₁₋₄-heteroaryl wherein the aryl or heteroaryl group is substituted or unsubstituted;

30

R² is selected from the group CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

35

R³ is selected from the group H, CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

aryl is phenyl substituted with 2-4 substituents
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl,
OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F,
5 CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,
-C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

heteroaryl is independently selected at each occurrence from
the group pyridyl, indolyl, benzothienyl,
10 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl,
2,3-dihydrobenzothienyl-S-oxide,
2,3-dihydrobenzothienyl-S-dioxide, indolinyl, and
benzoxazolin-2-on-yl, each heteroaryl being
substituted on 2-4 carbon atoms with a substituent
15 independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl,
OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F,
CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,
-C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each
20 heteroaryl being substituted on any nitrogen atom with
0-1 substituents selected from the group CH₃, CO₂CH₃,
COCH₃ and SO₂CH₃.

25 [4c] In another still more preferred embodiment, the present
invention provides a novel compound of formula Ic, wherein:

R¹ is substituted C₁;

30 R¹ is substituted with 0-1 substituents selected from the
group -CN, -CO₂CH₃, and -CO₂CH₂CH₃;

R¹ is also substituted with 0-2 substituents independently
selected at each occurrence from the group R^{1a}, R^{1b},
35 CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -
CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃,
F, CF₃, cyclopropyl, CH₃-cyclopropyl, cyclobutyl, CH₃-
cyclobutyl, cyclopentyl, CH₃-cyclopentyl;

R^{1a} is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, and OCF₃, and 0-2 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃, -CN, and SCH₃;

R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, and tetrazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, and SCH₃ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

provided that R¹ is other than a -(CH₂)₁₋₄-aryl or -(CH₂)₁₋₄-heteroaryl wherein the aryl or heteroaryl group is substituted or unsubstituted;

R² is selected from the group CH₃, CH₂CH₃, and CH(CH₃)₂;

R³ is selected from the group H and CH₃;

aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

heteroaryl is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃,

-NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and
-C(O)N(CH₃)₂.

5 [4d] In another further preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

R¹ is substituted (cyclopropyl)-C₁ alkyl or (cyclobutyl)C₁
alkyl;

10

R¹ is substituted with 0-1 -CN;

R¹ is also substituted with 0-1 substituents independently
selected at each occurrence from the group R^{1a}, R^{1b},
15 CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -
CH=CH(CH₃), -CH=CH, -CH=C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃,
F, CF₃, cyclopropyl, and CH₃-cyclopropyl;

20 R^{1a} is phenyl substituted with 0-1 substituents selected
from OCH₃, OCH₂CH₃, and OCF₃, and 0-2 substituents
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃,
-CN, and SCH₃;

25 R^{1b} is heteroaryl and is selected from the group furanyl,
thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl,
and pyrazolyl, each heteroaryl being substituted on
0-3 carbon atoms with a substituent independently
selected at each occurrence from the group CH₃, CH₂CH₃,
30 CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F,
CF₃, -CN, and SCH₃.

[4e] In another further preferred embodiment, the present
35 invention provides a novel compound of formula Ic, wherein:

R¹ is (cyclopropyl)C₁ alkyl or (cyclobutyl)-C₁ alkyl
substituted with 1 substituent independently selected

at each occurrence from the group R^{1a} , R^{1b} , CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $CH_2CH_2CH_3$, $-(CH_2)_3CH_3$, $-CH=CH_2$, $-CH=CH(CH_3)$, $-CH\equiv CH$, $-CH\equiv C(CH_3)$, $-CH_2OCH_3$, $-CH_2CH_2OCH_3$, F , CF_3 , cyclopropyl, and CH_3 -cyclopropyl;

5

R^{1a} is phenyl substituted with 0-2 substituents independently selected at each occurrence from the group CH_3 , CH_2CH_3 , Cl , F , and CF_3 ;

- 10 R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, and isoxazolyl, each heteroaryl being substituted on 0-2 carbon atoms with a substituent independently selected at each occurrence from the group CH_3 , OCH_3 , Cl , F , and CF_3 .

15

[4f] In an even further preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

- 20 R^1 is selected from the group (cyclopropyl) $CH-CH_3$, (cyclopropyl) $CH-CH_2CH_3$, (cyclopropyl) $CH-CH_2OCH_3$, (cyclopropyl) $CH-CH_2CH_2CH_3$, (cyclopropyl) $CH-CH_2CH_2OCH_3$, (cyclopropyl) $_2CH$, phenyl(cyclopropyl) CH , furanyl(cyclopropyl) CH , thienyl(cyclopropyl) CH ,
 25 isoxazolyl(cyclopropyl) CH , (CH_3 -furanyl)(cyclopropyl) CH , (cyclobutyl) $CH-CH_3$, (cyclobutyl) $CH-CH_2CH_3$, (cyclobutyl) $CH-CH_2OCH_3$, (cyclobutyl) $CH-CH_2CH_2CH_3$, (cyclobutyl) $CH-CH_2CH_2OCH_3$, (cyclobutyl) $_2CH$, phenyl(cyclobutyl) CH ,
 30 furanyl(cyclobutyl) CH , thienyl(cyclobutyl) CH , isoxazolyl(cyclobutyl) CH , and (CH_3 -furanyl)(cyclobutyl) CH ;

- 35 [4g] In another further preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

D is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

5

[4h] In another further preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

10 D is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

15

[4i] In another preferred embodiment, the present invention provides a novel compound of formula Ic, wherein the compound is selected from the group:

20

6-(2,4-bis(trifluoromethyl)phenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;

25 6-(2-chloro-4-cyanophenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;

6-(2-chloro-4-methoxy-5-chlorophenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;

30 6-(2-chloro-4-methoxy-5-methylphenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;

6-(2-chloro-4-methoxyphenyl)-8-ethyl-9-(2-hexyl)-9H-purine;

35 6-(2-chloro-4-methoxyphenyl)-8-ethyl-9-(2-pentyl)-9H-purine;

6-(2-chloro-4-methoxyphenyl)-8-ethyl-9-(3-heptyl)-9H-purine;

- 6-(2-chloro-4-methoxyphenyl)-8-ethyl-9-(3-hexyl)-9H-purine;
- 6-(2-chloro-4-methoxyphenyl)-8-ethyl-9-(4-heptyl)-9H-purine;
- 5 6-(2-chloro-4-methoxyphenyl)-9-(1-cyclopropylbutyl)-8-ethyl-9H-purine;
- 6-(2-chloro-4-methoxyphenyl)-9-(1-cyclopropylpropyl)-8-ethyl-9H-purine;
- 10 6-(2-chloro-4-methoxyphenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;
- 6-(2-chloro-4-methoxyphenyl)-9-(dicyclopropylmethyl)-8-methoxy-9H-purine;
- 15 6-(2-chloro-4-methyl-5-fluorophenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;
- 20 6-(2-chloro-4-methylphenyl)-8-ethyl-9-(2-pentyl)-9H-purine;
- 6-(2-chloro-4-methylphenyl)-8-ethyl-9-(4-heptyl)-9H-purine;
- 6-(2-chloro-4-methylphenyl)-9-(1-cyclopropylbutyl)-8-ethyl-9H-purine;
- 25 6-(2-chloro-4-methylphenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;
- 30 6-(2-chloro-4-trifluoromethoxyphenyl)-8-ethyl-9-(2-pentyl)-9H-purine;
- 6-(2-chloro-4-trifluoromethoxyphenyl)-8-ethyl-9-(3-hexyl)-9H-purine;
- 35 6-(2-chloro-4-trifluoromethoxyphenyl)-9-(1-cyclopropylbutyl)-8-ethyl-9H-purine;

- 6-(2-chloro-4-trifluoromethoxyphenyl)-9-(1-cyclopropylpropyl)-
8-ethyl-9H-purine;
- 5 6-(2-chloro-4-trifluoromethoxyphenyl)-9-(dicyclopropylmethyl)-
8-ethyl-9H-purine;
- 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-(1-hexyn-3-yl)-
9H-purine;
- 10 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-(1-pentyn-3-
yl)-9H-purine;
- 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-(1-pentyn-4-
yl)-9H-purine;
- 15 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-(1-phenyl-2-
butynyl)-9H-purine;
- 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-(2-heptyn-4-
yl)-9H-purine;
- 20 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-(2-hexyn-4-yl)-
9H-purine;
- 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-(2-pentyl)-9H-
purine;
- 25 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-(4-heptyl)-9H-
purine;
- 30 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-[(2-furanyl)-
cyclopropylmethyl]-9H-purine;
- 6-(2-chloro-4-trifluoromethylphenyl)-8-ethyl-9-[1-(2-
furanyl)propyl]-9H-purine;
- 35 6-(2-chloro-4-trifluoromethylphenyl)-9-(1-cyclobutylethyl)-8-
ethyl-9H-purine;

- 6-(2-chloro-4-trifluoromethylphenyl)-9-(1-cyclopropyl-2-butynyl)-8-ethyl-9H-purine;
- 5 6-(2-chloro-4-trifluoromethylphenyl)-9-(1-cyclopropyl-2-propenyl)-8-ethyl-9H-purine;
- 6-(2-chloro-4-trifluoromethylphenyl)-9-(1-cyclopropylbutyl)-8-ethyl-9H-purine;
- 10 6-(2-chloro-4-trifluoromethylphenyl)-9-(1-cyclopropylpropyl)-8-ethyl-9H-purine;
- 6-(2-chloro-4-trifluoromethylphenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;
- 15 8-ethyl-9H-purine;
- 6-(2-chloro-4-trifluoromethylphenyl)-9-(dicyclopropylmethyl)-8-methoxy-9H-purine;
- 20 6-(2-chloro-4-trifluoromethylphenyl)-9-[1-cyclopropyl-1-(2-thienyl)methyl]-8-ethyl-9H-purine;
- 9-(1-cyclobutylethyl)-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;
- 25 9-[1-cyclopropyl-(3-methylisoxazol-5-yl)methyl]-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;
- 9-(1-cyclopropyl-2-butynyl)-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;
- 30 9-(1-cyclopropyl-2-butynyl)-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;
- 9-(1-cyclopropyl-2-propenyl)-6-(2,4-dichloro-6-methylphenyl)-8-ethyl-9H-purine;
- 35 8-ethyl-9H-purine;

- 9-(1-cyclopropyl-2-propenyl)-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;
- 9-(1-cyclopropyl-2-propynyl)-8-ethyl-6-(2-trifluoromethyl-4-methoxyphenyl)-9H-purine;
- 9-(1-cyclopropyl-4'-fluorobenzyl)-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;
- 9-(1-cyclopropylbenzyl)-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;
- 9-(1-cyclopropylbenzyl)-8-ethyl-6-(2-trifluoromethyl-4-methoxyphenyl)-9H-purine;
- 9-(1-cyclopropylbutyl)-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;
- 9-(1-cyclopropylbutyl)-8-ethyl-6-(2,4,6-trimethylphenyl)-9H-purine;
- 9-(1-cyclopropylbutyl)-8-ethyl-6-(2-methyl-4,5-dimethoxyphenyl)-9H-purine;
- 9-(1-cyclopropylbutyl)-8-ethyl-6-(2-methyl-4-chlorophenyl)-9H-purine;
- 9-(1-cyclopropylbutyl)-8-ethyl-6-(2-methyl-4-methoxyphenyl)-9H-purine;
- 9-(1-cyclopropylbutyl)-8-ethyl-6-(2-trifluoromethyl-4-chlorophenyl)-9H-purine;
- 9-(1-cyclopropylbutyl)-8-ethyl-6-(2-trifluoromethyl-4-methoxyphenyl)-9H-purine;
- 9-(1-cyclopropylethyl)-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;

- 9-(1-cyclopropylethyl)-8-ethyl-6-(2-trifluoromethyl-4-chlorophenyl)-9H-purine;
- 5 9-(1-cyclopropylpentyl)-8-ethyl-6-(2-methyl-4-methoxyphenyl)-9H-purine;
- 9-(1-cyclopropylpropyl)-6-(2,4-dichloro-6-methylphenyl)-8-ethyl-9H-purine;
- 10 9-(1-cyclopropylpropyl)-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine;
- 9-(1-cyclopropylpropyl)-8-ethyl-6-(2,4,6-trimethylphenyl)-9H-purine;
- 15 9-(1-cyclopropylpropyl)-8-ethyl-6-(2-trifluoromethyl-4-chlorophenyl)-9H-purine;
- 20 6-(2,4-dichloro-5-fluorophenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;
- 6-(2,4-dichloro-6-methylphenyl)-8-ethyl-9-(2-penten-3-yl)-9H-purine;
- 25 6-(2,4-dichloro-6-methylphenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;
- 6-(2,4-dichlorophenyl)-8-ethyl-9-(1-hexyn-3-yl)-9H-purine;
- 30 6-(2,4-dichlorophenyl)-8-ethyl-9-(1-methoxycarbonylpropyl)-9H-purine;
- 6-(2,4-dichlorophenyl)-8-ethyl-9-(1-phenyl-2-butyryl)-9H-purine;
- 35 6-(2,4-dichlorophenyl)-8-ethyl-9-(2-heptyn-4-yl)-9H-purine;

- 6-(2,4-dichlorophenyl)-8-ethyl-9-(2-hexyl)-9H-purine;
- 6-(2,4-dichlorophenyl)-8-ethyl-9-(2-hexyn-4-yl)-9H-purine;
- 5 6-(2,4-dichlorophenyl)-8-ethyl-9-(2-penten-3-yl)-9H-purine;
- 6-(2,4-dichlorophenyl)-8-ethyl-9-(2-pentyl)-9H-purine;
- 6-(2,4-dichlorophenyl)-8-ethyl-9-(3-heptyl)-9H-purine;
- 10 6-(2,4-dichlorophenyl)-8-ethyl-9-(3-hexyl)-9H-purine;
- 6-(2,4-dichlorophenyl)-8-ethyl-9-(3-pentyl)-9H-purine;
- 15 6-(2,4-dichlorophenyl)-8-ethyl-9-(4-heptyl)-9H-purine;
- 6-(2,4-dichlorophenyl)-8-ethyl-9-[1-(2-methylcyclopropyl)ethyl]-9H-purine;
- 20 6-(2,4-dichlorophenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;
- 6-(2,4-dichlorophenyl)-9-(dicyclopropylmethyl)-8-ethyl-9H-purine;
- 25 6-(2,4-dichlorophenyl)-9-(dicyclopropylmethyl)-8-methoxy-9H-purine;
- 6-(2,4-dichlorophenyl)-9-(diphenylmethyl)-8-ethyl-9H-purine;
- 30 9-(dicyclopropylmethyl)-6-(2,4-dimethylphenyl)-8-ethyl-9H-purine;
- 9-(dicyclopropylmethyl)-6-(2,4-dimethylphenyl)-8-ethyl-9H-purine;
- 35 9-(dicyclopropylmethyl)-6-(2,6-dimethoxypyridin-3-yl)-8-methoxy-9H-purine;

- 9-(dicyclopropylmethyl)-8-ethyl-6-(2,4,5-trichlorophenyl)-9H-purine;
- 5 9-(dicyclopropylmethyl)-8-ethyl-6-(2-methoxy-4-trifluoromethylphenyl)-9H-purine;
- 9-(dicyclopropylmethyl)-8-ethyl-6-(2-methyl-4,5-dimethoxyphenyl)-9H-purine;
- 10 9-(dicyclopropylmethyl)-8-ethyl-6-(2-methyl-4-chlorophenyl)-9H-purine;
- 9-(dicyclopropylmethyl)-8-ethyl-6-(2-methyl-4-dimethylaminophenyl)-9H-purine;
- 15 9-(dicyclopropylmethyl)-8-ethyl-6-(2-methyl-4-methoxy-5-chlorophenyl)-9H-purine;
- 9-(dicyclopropylmethyl)-8-ethyl-6-(2-methyl-4-methoxy-5-fluorophenyl)-9H-purine;
- 20 9-(dicyclopropylmethyl)-8-ethyl-6-(2-chloro-4-methoxy-5-fluorophenyl)-9H-purine;
- 25 9-(dicyclopropylmethyl)-8-ethyl-6-(2-methyl-4-methoxyphenyl)-9H-purine;
- 9-(dicyclopropylmethyl)-8-ethyl-6-(2-trifluoromethyl-4-chlorophenyl)-9H-purine;
- 30 9-(dicyclopropylmethyl)-8-ethyl-6-(2-trifluoromethyl-4-methoxyphenyl)-9H-purine;
- 9-(dicyclopropylmethyl)-8-ethyl-6-(2-trifluoromethyl-4-propyloxyphenyl)-9H-purine;
- 35 6-(2,6-dimethoxypyridin-3-yl)-8-ethyl-9-(2-pentyl)-9H-purine;

- 6-(2,4-dimethylphenyl)-8-ethyl-9-(2-pentyl)-9H-purine;
- 5 8-ethyl-6-(2-methyl-4,5-dimethoxyphenyl)-9-(2-pentyl)-9H-purine;
- 8-ethyl-6-(2-methyl-4,5-dimethoxyphenyl)-9-(3-pentyl)-9H-purine;
- 10 8-ethyl-9-(1-hexen-3-yl)-6-(2-methyl-4,5-dimethoxyphenyl)-9H-purine;
- 8-ethyl-9-(1-hexen-3-yl)-6-(2-trifluoromethyl-4-methoxyphenyl)-9H-purine;
- 15 8-ethyl-9-(2-hexyl)-6-(2-trifluoromethyl-4-methoxyphenyl)-9H-purine;
- 8-ethyl-9-(2-pentyl)-6-(2-trifluoromethyl-4-methoxyphenyl)-9H-purine;
- 20 8-ethyl-9-(3-hexyl)-6-(2-methyl-4-methoxyphenyl)-9H-purine;
- 8-ethyl-9-(3-hexyl)-6-(2-trifluoromethyl-4-methoxyphenyl)-9H-purine;
- 25 8-ethyl-9-(3-pentyl)-6-(2-trifluoromethyl-4-chlorophenyl)-9H-purine;
- 8-ethyl-9-(4-heptyl)-6-(2-methyl-4-chlorophenyl)-9H-purine;
- 30 8-ethyl-9-(4-heptyl)-6-(2-methyl-4-methoxyphenyl)-9H-purine;
- 8-ethyl-9-(4-heptyl)-6-(2-trifluoromethyl-4-chlorophenyl)-9H-purine;
- 35 8-ethyl-9-(4-heptyl)-6-(2-trifluoromethyl-4 methoxyphenyl)-9H-purine; and

9-(dicyclopropylmethyl)-8-ethyl-6-(2-methyl-6-methoxy-3-pyridyl)-9H-purine;

5 or a pharmaceutically acceptable salt form thereof.

[4j] In another more preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

10

R¹ is C₃₋₈ cycloalkyl;

R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, -NR^{15a}COR^{13a},
15 -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b},
-CONR^{13a}R^{16a}, 1-morpholinyl, 1-piperidinyl, 1-piperazinyl, and C₄₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O⁻, -S(O)_n⁻, -NR^{13a}⁻,
20 -NCO₂R^{14b}⁻, -NCOR^{14b}⁻ and -NSO₂R^{14b}⁻, and wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b}; and,

25 R¹ is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, R^{1c}, C₁₋₆ alkyl, C₂₋₉ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -OR^{13a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and -NR^{13a}R^{16a}.

30

[4k] In another even more preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

35 X is selected from the group O, S(O)_n and a bond;

n is 0, 1 or 2;

- R^1 is selected from the group cyclopropyl, cyclobutyl, and cyclopentyl;
- 5 R^1 is substituted with 0-1 substituents selected from the group -CN, $-S(O)_nR^{14b}$, $-COR^{13a}$, $-CO_2R^{13a}$, and C_{4-8} cycloalkyl, wherein one carbon atom in the C_{4-8} cycloalkyl is replaced by a group selected from the group -O-, $-S(O)_n$ -, $-NR^{13a}$ -, $-NCO_2R^{14b}$ -, $-NCOR^{14b}$ - and
- 10 $-NSO_2R^{14b}$ -;
- R^1 is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a} , R^{1b} , C_{1-6} alkyl, C_{2-8} alkenyl, C_{2-8} alkynyl, Br, Cl, F, CF_3 ,
- 15 CF_2CF_3 , $-OR^{13a}$, C_{1-2} alkoxy- C_{1-2} alkyl, and $-NR^{13a}R^{16a}$;
- R^{1a} is aryl and is selected from the group phenyl and indanyl, each R^{1a} being substituted with 0-1 $-OR^{17}$ and
- 20 0-5 substituents independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, C_{1-4} haloalkyl, -CN, $-S(O)_mR^{18}$, $-COR^{17}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$;
- R^{1b} is heteroaryl and is selected from the group pyridyl,
- 25 pyrimidinyl, furanyl, thienyl, imidazolyl, thiazolyl, pyrrolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the
- 30 group C_{1-4} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, CF_3 , -CN, $-OR^{17}$, $-S(O)_mR^{18}$, $-COR^{17}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group
- R^{15a} , CO_2R^{14b} , COR^{14b} and SO_2R^{14b} ;
- 35 R^2 is selected from the group C_{1-4} alkyl, C_{2-4} alkenyl, and C_{2-4} alkynyl and is substituted with 0-1 substituents

selected from the group -CN, OH, Cl, F, and C₁₋₄ alkoxy;

5 R⁹ is independently selected at each occurrence from the group H, C₁₋₄ alkyl and C₃₋₈ cycloalkyl;

R³ is selected from the group H, Br, Cl, F, -CN, C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₁₋₄ alkoxy, NH₂, C₁₋₄ alkylamino, and (C₁₋₄ alkyl)₂-amino;

10

R¹³ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;

15 R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

20 R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl, aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;

25 R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;

R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;

30

R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, C₁₋₄ haloalkyl, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

35

- R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 5 R¹⁷, R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;
- 10 alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;
- 15 R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ haloalkyl;
- 20 aryl is phenyl substituted with 1-4 substituents independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, -OR¹⁷, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷, -CO₂R¹⁷, -NR¹⁵COR¹⁷, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹; and,
- 25 heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, 30 benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 1-4 carbon atoms with a substituent independently selected
- 35

at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and
5 each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and SO₂R^{14a}.

10 [41] In another still more preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

X is selected from the group O, S and a bond;

15 R¹ is substituted with 0-1 substituents selected from the group -CN, -CO₂R^{13a}, and C₄₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;

20 R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃, CF₃, -OR^{13a}, -OH, -OCH₃, -OCH₂CH₃, -CH₂OCH₃, -
25 CH₂CH₂OCH₃, and -NR^{13a}R^{16a};

R^{1a} is aryl and is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-3 substituents independently selected at
30 each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂;

35 R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each

heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂,
5 OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

10

R² is selected from the group CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

15

R³ is selected from the group H, CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

20

aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

25

heteroaryl is independently selected at each occurrence from the group pyridyl, indolyl, benzothienyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, and benzoxazolin-2-on-yl, each heteroaryl being

30

substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,

35

-C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃.

[4m] In another further preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

- 5
R¹ is substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃,
10 F, and CF₃;
- R^{1a} is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-2 substituents independently selected at each
15 occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃, -CN, and SCH₃;
- R^{1b} is heteroaryl and is selected from the group furanyl, thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl,
20 pyrazolyl, triazolyl, and tetrazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, and SCH₃ and each
25 heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;
- R² is selected from the group CH₃, CH₂CH₃, and CH(CH₃)₂;
- 30 R³ is selected from the group H and CH₃;
- aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the
35 group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

heteroaryl is pyridyl substituted on 2-4 carbon atoms with
a substituent independently selected at each
occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂,
5 CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂,
OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃,
-NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and
-C(O)N(CH₃)₂.

10

[4n] In another even further preferred embodiment, the present
invention provides a novel compound of formula Ic, wherein:

15 R¹ is substituted with 0-2 substituents independently
selected at each occurrence from the group R^{1a}, CH₃,
CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH₂OCH₃, -
CH₂CH₂OCH₃, F, and CF₃; and,

20 R^{1a} is phenyl substituted with 0-2 substituents
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃,
-CN, and SCH₃.

25 [4o] In another still further preferred embodiment, the
present invention provides a novel compound of formula Ic,
wherein:

30 D is phenyl substituted with 2-4 substituents independently
selected at each occurrence from the group CH₃, CH₂CH₃,
CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃,
OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

35 [4p] In another still further preferred embodiment, the
present invention provides a novel compound of formula Ic,
wherein:

D is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃,
5 Br, Cl, F, and CF₃.

[4q] In another more preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

10

R¹ is selected from the group C₁₋₁₀ alkyl, C₂₋₁₀ alkenyl, C₂₋₁₀ alkynyl, C₃₋₈ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ alkoxy-C₁₋₄ alkyl;

15 R¹ is substituted with a C₃₋₈ cycloalkyl group, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl group is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-;

20 R¹ is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, R^{1c}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₈ cycloalkyl which is substituted with 0-
25 1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;

30 R^{1a} is aryl and is selected from the group phenyl, naphthyl, indanyl and indenyl, each R^{1a} being substituted with 0-1 -OR¹⁷ and 0-5 substituents independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro,
35 SH, -S(O)_nR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂, -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a};

R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-onyl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, -CN, nitro, $-OR^{17}$, SH, $-S(O)_mR^{18}$, $-COR^{17}$, $-OC(O)R^{18}$, $-NR^{15a}COR^{17}$, $-N(COR^{17})_2$, $-NR^{15a}CONR^{17a}R^{19a}$, $-NR^{15a}CO_2R^{18}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15a} , CO_2R^{14b} , COR^{14b} and SO_2R^{14b} ; and,

R^{1c} is heterocyclyl and is a saturated or partially saturated heteroaryl, each heterocyclyl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, -CN, nitro, $-OR^{13a}$, SH, $-S(O)_nR^{14b}$, $-COR^{13a}$, $-OC(O)R^{14b}$, $-NR^{15a}COR^{13a}$, $-N(COR^{13a})_2$, $-NR^{15a}CONR^{13a}R^{16a}$, $-NR^{15a}CO_2R^{14b}$, $-NR^{13a}R^{16a}$, and $-CONR^{13a}R^{16a}$ and each heterocyclyl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{13a} , CO_2R^{14b} , COR^{14b} and SO_2R^{14b} and wherein any sulfur atom is optionally monooxidized or dioxidized.

35

[4r] In another even more preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

X is selected from the group O, S(O)_n and a bond;

5

n is 0, 1 or 2;

R¹ is selected from the group C₁₋₆ alkyl, C₂₋₆ alkenyl, C₂₋₆ alkynyl, and C₃₋₈ cycloalkyl;

10

R¹ is substituted with a C₃₋₆ cycloalkyl group, wherein 0-1 carbon atoms in the C₄₋₆ cycloalkyl group is replaced by a group selected from the group -O-, -S(O)_n-, and -NR^{13a}-;

15

R¹ is also substituted with 0-2 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, CF₃, CF₂CF₃, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

20

R^{1a} is aryl and is selected from the group phenyl and indanyl, each R^{1a} being substituted with 0-1 -OR¹⁷ and 0-5 substituents independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -S(O)_nR¹⁸, -COR¹⁷, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a};

25

30

R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, furanyl, thienyl, imidazolyl, thiazolyl, pyrrolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₄ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, CF₃, -CN,

35

-OR¹⁷, -S(O)_mR¹⁸, -COR¹⁷, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a}
and each heteroaryl being substituted on any nitrogen
atom with 0-1 substituents selected from the group
R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

5

R² is selected from the group C₁₋₄ alkyl, C₂₋₄ alkenyl, and
C₂₋₄ alkynyl and is substituted with 0-1 substituents
selected from the group -CN, OH, Cl, F, and C₁₋₄
alkoxy;

10

R⁹ is independently selected at each occurrence from the
group H, C₁₋₄ alkyl and C₃₋₈ cycloalkyl;

R³ is selected from the group H, Br, Cl, F, -CN, C₁₋₄ alkyl,
15 C₃₋₆ cycloalkyl, C₁₋₄ alkoxy, NH₂, C₁₋₄ alkylamino, and
(C₁₋₄ alkyl)₂-amino;

R¹³ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl,
C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl,
20 aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;

R^{13a} and R^{16a} are independently selected at each occurrence
from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄
alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-
25 C₁₋₆ alkyl;

R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl,
C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl-C₁₋₂ alkyl,
aryl(C₁₋₂ alkyl)-, and heteroaryl(C₁₋₂ alkyl)-;

30

R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl,
C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₃₋₆ cycloalkyl-C₁₋₂ alkyl;

R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₂ haloalkyl,
35 C₁₋₂ alkoxy-C₁₋₂ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆
cycloalkyl-C₁₋₂ alkyl;

5 R^{15} is independently selected at each occurrence from the group H, C_{1-4} alkyl, C_{3-7} cycloalkyl, C_{3-6} cycloalkyl- C_{1-6} alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C_{1-4} alkyl, Br, Cl, F, C_{1-4} haloalkyl, C_{1-4} alkoxy, C_{1-4} haloalkoxy, and dimethylamino;

10 R^{15a} is independently selected at each occurrence from the group H, C_{1-4} alkyl, C_{3-7} cycloalkyl, and C_{3-6} cycloalkyl- C_{1-6} alkyl;

15 R^{17} , R^{18} and R^{19} are independently selected at each occurrence from the group H, C_{1-6} alkyl, C_{3-10} cycloalkyl, C_{3-6} cycloalkyl- C_{1-6} alkyl, C_{1-2} alkoxy- C_{1-2} alkyl, and C_{1-4} haloalkyl;

20 alternatively, in an $NR^{17}R^{19}$ moiety, R^{17} and R^{19} taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N_4 in 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13} , CO_2R^{14} , COR^{14} and SO_2R^{14} ;

25 R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C_{1-6} alkyl, C_{3-10} cycloalkyl, C_{3-6} cycloalkyl- C_{1-6} alkyl and C_{1-4} haloalkyl;

30 aryl is phenyl substituted with 1-4 substituents independently selected at each occurrence from the group C_{1-4} alkyl, C_{3-6} cycloalkyl, $-OR^{17}$, Br, Cl, F, C_{1-4} haloalkyl, $-CN$, $-S(O)_nR^{18}$, $-COR^{17}$, $-CO_2R^{17}$, $-NR^{15}COR^{17}$, $-NR^{15}CO_2R^{18}$, $-NR^{17}R^{19}$, and $-CONR^{17}R^{19}$; and,

35 heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl,

benzothienyl, benzothiazolyl, benzoxazolyl,
 isoxazolyl, tetrazolyl, indazolyl,
 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl,
 2,3-dihydrobenzothienyl-S-oxide,
 5 2,3-dihydrobenzothienyl-S-dioxide, indoliny,
 benzoxazolin-2-on-yl, benzodioxolanyl and
 benzodioxane, each heteroaryl being substituted 1-4
 carbon atoms with a substituent independently selected
 at each occurrence from the group C₁₋₆ alkyl, C₃₋₆
 10 cycloalkyl, Br, Cl, F, C₁₋₄ haloalkyl, -CN, -OR¹⁷,
 -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷,
 -N(COR¹⁷)₂, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and
 each heteroaryl being substituted on any nitrogen atom
 with 0-1 substituents selected from the group R¹⁵,
 15 CO₂R^{14a}, COR^{14a} and SO₂R^{14a}.

[4s] In another still more preferred embodiment, the present
 invention provides a novel compound of formula Ic, wherein:

20

X is selected from the group O, S and a bond;

R¹ is C₁₋₆ alkyl;

25 R¹ is substituted with a C₃₋₆ cycloalkyl, wherein 0-1 carbon
 atoms in the C₄₋₄ cycloalkyl is replaced by a group
 selected from the group -O-, -S(O)_n-, and -NR^{13a}-;

30 R¹ is also substituted with 0-2 substituents independently
 selected at each occurrence from the group R^{1a}, R^{1b},
 C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, F, CF₃, -OR^{13a},
 -NR^{13a}R^{16a}, -CH₂OCH₃, -CH₂CH₂OCH₃, and C₃₋₆ cycloalkyl
 which is substituted with 0-1 CH₃ and in which 0-1
 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

35

provided that R¹ is other than a cyclohexyl-(CH₂)₂- group;

R^{1a} is aryl and is phenyl substituted with 0-1 substituents selected from OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, and OCF₃, and 0-3 substituents independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂,
5 CH₂CH₂CH₃, cyclopropyl, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂;

R^{1b} is heteroaryl and is selected from the group furanyl,
10 thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, and indazolyl, each heteroaryl being substituted on 0-3 carbon atoms with a substituent independently selected at each occurrence from the group CH₃, CH₂CH₃, CH(CH₃)₂,
15 CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group
20 CH₃, CO₂CH₃, COCH₃ and SO₂CH₃;

R² is selected from the group CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

25 R³ is selected from the group H, CH₃, CH₂CH₃, CH(CH₃)₂, and CH₂CH₂CH₃;

aryl is phenyl substituted with 2-4 substituents independently selected at each occurrence from the
30 group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂; and,

35 heteroaryl is independently selected at each occurrence from the group pyridyl, indolyl, benzothienyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide,

2,3-dihydrobenzothienyl-S-dioxide, indoliny1, and
benzoxazolin-2-on-yl, each heteroaryl being
substituted on 2-4 carbon atoms with a substituent
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl,
OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F,
CF₃, -CN, SCH₃, SO₂CH₃, -NH₂, -NHCH₃, -N(CH₃)₂,
-C(O)NH₂, -C(O)NHCH₃, and -C(O)N(CH₃)₂ and each
heteroaryl being substituted on any nitrogen atom with
0-1 substituents selected from the group CH₃, CO₂CH₃,
COCH₃ and SO₂CH₃.

[4t] In another further preferred embodiment, the present
invention provides a novel compound of formula Ic, wherein:

R¹ is (cyclopropyl)C₁ alkyl or (cyclobutyl)C₁ alkyl;

R¹ is substituted with 1-2 substituents independently
selected at each occurrence from the group R^{1a}, R^{1b},
CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, -(CH₂)₃CH₃, -CH=CH₂, -
CH=CH(CH₃), -CH≡CH, -CH≡C(CH₃), -CH₂OCH₃, -CH₂CH₂OCH₃,
F, CF₃, cyclopropyl, CH₃-cyclopropyl, cyclobutyl, CH₃-
cyclobutyl, cyclopentyl, CH₃-cyclopentyl;

R^{1a} is phenyl substituted with 0-1 substituents selected
from OCH₃, OCH₂CH₃, and OCF₃, and 0-2 substituents
independently selected at each occurrence from the
group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃,
-CN, and SCH₃;

R^{1b} is heteroaryl and is selected from the group furanyl,
thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl,
pyrazolyl, triazolyl, and tetrazolyl, each heteroaryl
being substituted on 0-3 carbon atoms with a
substituent independently selected at each occurrence
from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, OCH₃,
OCH₂CH₃, OCF₃, Br, Cl, F, CF₃, -CN, and SCH₃ and each

heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group CH_3 , CO_2CH_3 , COCH_3 and SO_2CH_3 ;

5 R^2 is selected from the group CH_3 , CH_2CH_3 , and $\text{CH}(\text{CH}_3)_2$;

R^3 is selected from the group H and CH_3 ;

aryl is phenyl substituted with 2-4 substituents

10 independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, cyclopropyl, OCH_3 , OCH_2CH_3 , $\text{OCH}(\text{CH}_3)_2$, $\text{OCH}_2\text{CH}_2\text{CH}_3$, OCF_3 , Br, Cl, F, CF_3 , $-\text{CN}$, SCH_3 , SO_2CH_3 , $-\text{NH}_2$, $-\text{NHCH}_3$, $-\text{N}(\text{CH}_3)_2$, $-\text{C}(\text{O})\text{NH}_2$, $-\text{C}(\text{O})\text{NHCH}_3$, and $-\text{C}(\text{O})\text{N}(\text{CH}_3)_2$; and,

15

heteroaryl is pyridyl substituted on 2-4 carbon atoms with a substituent independently selected at each occurrence from the group CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, cyclopropyl, OCH_3 , OCH_2CH_3 , $\text{OCH}(\text{CH}_3)_2$, $\text{OCH}_2\text{CH}_2\text{CH}_3$, OCF_3 , Br, Cl, F, CF_3 , $-\text{CN}$, SCH_3 , SO_2CH_3 , $-\text{NH}_2$, $-\text{NHCH}_3$, $-\text{N}(\text{CH}_3)_2$, $-\text{C}(\text{O})\text{NH}_2$, $-\text{C}(\text{O})\text{NHCH}_3$, and $-\text{C}(\text{O})\text{N}(\text{CH}_3)_2$.

20

25 [4u] In another even further preferred embodiment, the present invention provides a novel compound of formula Ic, wherein:

R^1 is (cyclopropyl) C_1 alkyl or (cyclobutyl) C_1 alkyl;

30

R^1 is substituted with 1-2 substituents independently selected at each occurrence from the group R^{1a} , R^{1b} , CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{CH}_2\text{CH}_2\text{CH}_3$, $-(\text{CH}_2)_3\text{CH}_3$, $-\text{CH}=\text{CH}_2$, $-\text{CH}=\text{CH}(\text{CH}_3)$, $-\text{CH}=\text{CH}$, $-\text{CH}=\text{C}(\text{CH}_3)$, $-\text{CH}_2\text{OCH}_3$, $-\text{CH}_2\text{CH}_2\text{OCH}_3$, F, CF_3 , cyclopropyl, and CH_3 -cyclopropyl;

35

R^{1a} is phenyl substituted with 0-2 substituents independently selected at each occurrence from the

group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃, Br, Cl, F, CF₃,
-CN, and SCH₃;

5 R^{1b} is heteroaryl and is selected from the group furanyl,
thienyl, imidazolyl, thiazolyl, oxazolyl, isoxazolyl,
and pyrazolyl, each heteroaryl being substituted on
0-3 carbon atoms with a substituent independently
selected at each occurrence from the group CH₃, CH₂CH₃,
CH(CH₃)₂, CH₂CH₂CH₃, OCH₃, OCH₂CH₃, OCF₃, Br, Cl, F,
10 CF₃, -CN, and SCH₃.

[4v] In another further preferred embodiment, the present
invention provides a novel compound of formula Ic, wherein:

15 D is phenyl substituted with 2-4 substituents independently
selected at each occurrence from the group CH₃, CH₂CH₃,
CH(CH₃)₂, CH₂CH₂CH₃, cyclopropyl, OCH₃, OCH₂CH₃,
OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃, Br, Cl, F, and CF₃.

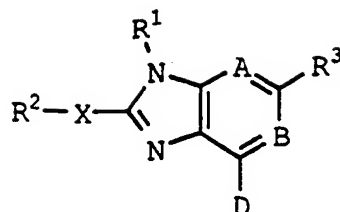
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[4w] In another further preferred embodiment, the present
invention provides a novel compound of formula Ic, wherein:

25 D is pyridyl substituted on 2-4 carbon atoms with a
substituent independently selected at each occurrence
from the group CH₃, CH₂CH₃, CH(CH₃)₂, CH₂CH₂CH₃,
cyclopropyl, OCH₃, OCH₂CH₃, OCH(CH₃)₂, OCH₂CH₂CH₃, OCF₃,
Br, Cl, F, and CF₃.

30

[5] In a third embodiment, the present invention provides
a novel pharmaceutical composition, comprising: a
pharmaceutically acceptable carrier and a
35 therapeutically effective amount of a compound of
formula (I):



(I)

or a stereoisomer or pharmaceutically acceptable salt form thereof, wherein:

5

A is N or C-R⁷;

B is N or C-R⁸;

10 provided that at least one of the groups A and B is N;

D is an aryl or heteroaryl group attached through an unsaturated carbon atom;

15 X is selected from the group CH-R⁹, N-R¹⁰, O, S(O)_n and a bond;

n is 0, 1 or 2;

20 R¹ is selected from the group C₁₋₁₀ alkyl, C₂₋₁₀ alkenyl, C₂₋₁₀ alkynyl, C₃₋₈ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, -SO₂-C₁₋₁₀ alkyl, -SO₂-R^{1a}, and -SO₂-R^{1b};

25 R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b}, -CONR^{13a}R^{16a}, 1-morpholinyl, 1-piperidinyl, 1-piperazinyl, and C₃₋₈ cycloalkyl, wherein 0-1 carbon
30 atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-, and wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents

selected from the group R^{13a} , CO_2R^{14b} , COR^{14b} and SO_2R^{14b} ;

5 R^1 is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a} , R^{1b} , R^{1c} , C_{1-6} alkyl, C_{2-8} alkenyl, C_{2-8} alkynyl, Br, Cl, F, I, C_{1-4} haloalkyl, $-OR^{13a}$, $-NR^{13a}R^{16a}$, and C_{3-8} cycloalkyl which is substituted with 0-1 R^9 and in which 0-1 carbons of C_{4-8} cycloalkyl is replaced by
10 $-O-$;

provided that R^1 is other than:

- (a) a 3-cyclopropyl-3-methoxypropyl group;
- (b) an unsubstituted-(alkoxy)methyl group; and,
- 15 (c) a 1-hydroxyalkyl group;

also provided that when R^1 alkyl substituted with OH, then the carbon adjacent to the ring N is other than CH_2 ;

20 R^{1a} is aryl and is selected from the group phenyl, naphthyl, indanyl and indenyl, each R^{1a} being substituted with 0-5 substituents independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, $-CN$, nitro, $-OR^{17}$, SH,
25 $-S(O)_nR^{18}$, $-COR^{17}$, $-OC(O)R^{18}$, $-NR^{15a}COR^{17}$, $-N(COR^{17})_2$, $-NR^{15a}CONR^{17a}R^{19a}$, $-NR^{15a}CO_2R^{18}$, $-NR^{17a}R^{19a}$, and $-CONR^{17a}R^{19a}$;

R^{1b} is heteroaryl and is selected from the group pyridyl,
30 pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl,
35 indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide,

2,3-dihydrobenzothienyl-S-dioxide, indoliny, benzoxazolin-2-onyl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH, -S(O)_mR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂, -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a} and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

R^{1c} is heterocyclyl and is a saturated or partially saturated heteroaryl, each heterocyclyl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR^{13a}, SH, -S(O)_nR^{14b}, -COR^{13a}, -OC(O)R^{14b}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b}, -NR^{13a}R^{16a}, and -CONR^{13a}R^{16a} and each heterocyclyl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b} and wherein any sulfur atom is optionally monooxidized or dioxidized;

R² is selected from the group C₁₋₄ alkyl, C₃₋₈ cycloalkyl, C₂₋₄ alkenyl, and C₂₋₄ alkynyl and is substituted with 0-3 substituents selected from the group -CN, hydroxy, halo and C₁₋₄ alkoxy;

alternatively R², in the case where X is a bond, is selected from the group -CN, CF₃ and C₂F₅;

R³, R⁷ and R⁸ are independently selected at each occurrence from the group H, Br, Cl, F, I, -CN, C₁₋₄ alkyl, C₃₋₈ cycloalkyl, C₁₋₄ alkoxy, C₁₋₄ alkylthio, C₁₋₄ alkylsulfinyl, C₁₋₄ alkylsulfonyl, amino, C₁₋₄

alkylamino, (C₁₋₄ alkyl)₂amino and phenyl, each phenyl is substituted with 0-3 groups selected from the group C₁₋₇ alkyl, C₃₋₈ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, C₁₋₄ alkylthio, C₁₋₄ alkyl sulfinyl, C₁₋₄ alkylsulfonyl, C₁₋₆ alkylamino and (C₁₋₄ alkyl)₂amino;

provided that when R¹ is unsubstituted C₁₋₁₀ alkyl, then R³ is other than substituted or unsubstituted phenyl;

10

R⁹ and R¹⁰ are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₆ cycloalkyl-C₁₋₄ alkyl and C₃₋₈ cycloalkyl;

15 R¹³ is selected from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)-;

20 R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

25 R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)- and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy C₁₋₄ haloalkoxy, and dimethylamino;

30 R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄

haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

5 R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

10 R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

15 R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

20 R¹⁷ is selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₁₋₄ haloalkyl, R¹⁴S(O)_n-C₁₋₄ alkyl, and R^{17b}R^{19b}N-C₂₋₄ alkyl;

25 R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;

30 alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;

35 alternatively, in an NR^{17b}R^{19b} moiety, R^{17b} and R^{19b} taken together form 1-pyrrolidinyl, 1-morpholinyl,

1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;

- 5 R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ haloalkyl;

- 10 aryl is independently selected at each occurrence from the group phenyl, naphthyl, indanyl and indenyl, each aryl being substituted with 0-5 substituents independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, methylenedioxy, C₁₋₄ alkoxy-C₁₋₄ alkoxy, -OR¹⁷, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, -NO₂,
15 SH, -S(O)_nR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CONR¹⁷R¹⁹, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and up to 1 phenyl, each phenyl substituent being substituted with 0-4 substituents selected from the group C₁₋₃ alkyl, C₁₋₃ alkoxy, Br, Cl, F, I, -CN,
20 dimethylamino, CF₃, C₂F₅, OCF₃, SO₂Me and acetyl; and,

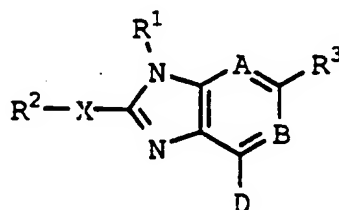
- heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl,
25 thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, triazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide,
30 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆
35 cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH, -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CONR¹⁷R¹⁹, -NR¹⁵CO₂R¹⁸,

-NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and SO₂R^{14a}.

5

- [6] In a second embodiment, the present invention provides a novel method of treating affective disorder, anxiety, depression, headache, irritable bowel syndrome, post-traumatic stress disorder, supranuclear palsy, immune suppression, Alzheimer's disease, gastrointestinal diseases, anorexia nervosa or other feeding disorder, drug addiction, drug or alcohol withdrawal symptoms, inflammatory diseases, cardiovascular or heart-related diseases, fertility problems, human immunodeficiency virus infections, hemorrhagic stress, obesity, infertility, head and spinal cord traumas, epilepsy, stroke, ulcers, amyotrophic lateral sclerosis, hypoglycemia or a disorder the treatment of which can be effected or facilitated by antagonizing CRF, including but not limited to disorders induced or facilitated by CRF, in mammals, comprising: administering to the mammal a therapeutically effective amount of a compound of formula (I):

25



(I)

or a stereoisomer or pharmaceutically acceptable salt form thereof, wherein:

30

A is N or C-R⁷;

B is N or C-R⁸;

provided that at least one of the groups A and B is N;

D is an aryl or heteroaryl group attached through an unsaturated carbon atom;

5

X is selected from the group CH-R⁹, N-R¹⁰, O, S(O)_n and a bond;

n is 0, 1 or 2;

10

R¹ is selected from the group C₁₋₁₀ alkyl, C₂₋₁₀ alkenyl, C₂₋₁₀ alkynyl, C₃₋₈ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, -SO₂-C₁₋₁₀ alkyl, -SO₂-R^{1a}, and -SO₂-R^{1b};

15

R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b}, -CONR^{13a}R^{16a}, 1-morpholinyl, 1-piperidinyl, 1-piperazinyl, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-, and wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

20

25

R¹ is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, R^{1c}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -OR^{13a}, -NR^{13a}R^{16a}, and C₃₋₈ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

30

35

provided that R¹ is other than:

(a) a 3-cyclopropyl-3-methoxypropyl group;

- (b) an unsubstituted-(alkoxy)methyl group; and,
- (c) a 1-hydroxyalkyl group;

also provided that when R¹ alkyl substituted with OH, then
 5 the carbon adjacent to the ring N is other than CH₂;

R^{1a} is aryl and is selected from the group phenyl, naphthyl,
 indanyl and indenyl, each R^{1a} being substituted with
 0-5 substituents independently selected at each
 10 occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl,
 Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH,
 -S(O)_nR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂,
 -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and
 -CONR^{17a}R^{19a};

15 R^{1b} is heteroaryl and is selected from the group pyridyl,
 pyrimidinyl, triazinyl, furanyl, quinolinyl,
 isoquinolinyl, thienyl, imidazolyl, thiazolyl,
 indolyl, pyrrolyl, oxazolyl, benzofuranyl,
 20 benzothienyl, benzothiazolyl, benzoxazolyl,
 isoxazolyl, pyrazolyl, triazolyl, tetrazolyl,
 indazolyl, 2,3-dihydrobenzofuranyl,
 2,3-dihydrobenzothienyl,
 2,3-dihydrobenzothienyl-S-oxide,
 25 2,3-dihydrobenzothienyl-S-dioxide, indolinyl,
 benzoxazolin-2-onyl, benzodioxolanyl and benzodioxane,
 each heteroaryl being substituted on 0-4 carbon atoms
 with a substituent independently selected at each
 occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl,
 30 Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH,
 -S(O)_mR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂,
 -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and
 -CONR^{17a}R^{19a} and each heteroaryl being substituted on
 any nitrogen atom with 0-1 substituents selected from
 35 the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

- R^{1c} is heterocyclyl and is a saturated or partially saturated heteroaryl, each heterocyclyl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, -CN, nitro, $-OR^{13a}$, SH, $-S(O)_nR^{14b}$, $-COR^{13a}$, $-OC(O)R^{14b}$, $-NR^{15a}COR^{13a}$, $-N(COR^{13a})_2$, $-NR^{15a}CONR^{13a}R^{16a}$, $-NR^{15a}CO_2R^{14b}$, $-NR^{13a}R^{16a}$, and $-CONR^{13a}R^{16a}$ and each heterocyclyl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{13a} , CO_2R^{14b} , COR^{14b} and SO_2R^{14b} and wherein any sulfur atom is optionally monooxidized or dioxidized;
- R^2 is selected from the group C_{1-4} alkyl, C_{3-8} cycloalkyl, C_{2-4} alkenyl, and C_{2-4} alkynyl and is substituted with 0-3 substituents selected from the group -CN, hydroxy, halo and C_{1-4} alkoxy;
- alternatively R^2 , in the case where X is a bond, is selected from the group -CN, CF_3 and C_2F_5 ;
- R^3 , R^7 and R^8 are independently selected at each occurrence from the group H, Br, Cl, F, I, -CN, C_{1-4} alkyl, C_{3-8} cycloalkyl, C_{1-4} alkoxy, C_{1-4} alkylthio, C_{1-4} alkylsulfinyl, C_{1-4} alkylsulfonyl, amino, C_{1-4} alkylamino, $(C_{1-4} \text{ alkyl})_2\text{amino}$ and phenyl, each phenyl is substituted with 0-3 groups selected from the group C_{1-7} alkyl, C_{3-8} cycloalkyl, Br, Cl, F, I, C_{1-4} haloalkyl, nitro, C_{1-4} alkoxy, C_{1-4} haloalkoxy, C_{1-4} alkylthio, C_{1-4} alkyl sulfinyl, C_{1-4} alkylsulfonyl, C_{1-6} alkylamino and $(C_{1-4} \text{ alkyl})_2\text{amino}$;
- provided that when R^1 is unsubstituted C_{1-10} alkyl, then R^3 is other than substituted or unsubstituted phenyl;

- R⁹ and R¹⁰ are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₆ cycloalkyl-C₁₋₄ alkyl and C₃₋₈ cycloalkyl;
- 5 R¹³ is selected from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)-;
- 10 R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 15 R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)- and benzyl, each benzyl being substituted on the aryl moiety with 0-1
- 20 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy C₁₋₄ haloalkoxy, and dimethylamino;
- R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and
- 25 dimethylamino;
- 30 R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;
- 35 R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl

being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

5

R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

10 R¹⁷ is selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₁₋₄ haloalkyl, R¹⁴S(O)_n-C₁₋₄ alkyl, and R^{17b}R^{19b}N-C₂₋₄ alkyl;

15 R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;

20 alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;

25

alternatively, in an NR^{17b}R^{19b} moiety, R^{17b} and R^{19b} taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents
30 selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;

R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ haloalkyl;

35

aryl is independently selected at each occurrence from the group phenyl, naphthyl, indanyl and indenyl, each aryl

being substituted with 0-5 substituents independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, methylenedioxy, C₁₋₄ alkoxy-C₁₋₄ alkoxy, -OR¹⁷, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, -NO₂,
 5 SH, -S(O)_nR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷,
 -N(COR¹⁷)₂, -NR¹⁵CONR¹⁷R¹⁹, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and
 -CONR¹⁷R¹⁹ and up to 1 phenyl, each phenyl substituent
 being substituted with 0-4 substituents selected from
 the group C₁₋₃ alkyl, C₁₋₃ alkoxy, Br, Cl, F, I, -CN,
 10 dimethylamino, CF₃, C₂F₅, OCF₃, SO₂Me and acetyl; and,

heteroaryl is independently selected at each occurrence from
 the group pyridyl, pyrimidinyl, triazinyl, furanyl,
 quinolinyl, isoquinolinyl, thienyl, imidazolyl,
 15 thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl,
 benzothienyl, benzothiazolyl, benzoxazolyl,
 isoxazolyl, triazolyl, tetrazolyl, indazolyl,
 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl,
 2,3-dihydrobenzothienyl-S-oxide,
 20 2,3-dihydrobenzothienyl-S-dioxide, indolinyl,
 benzoxazolin-2-on-yl, benzodioxolanyl and
 benzodioxane, each heteroaryl being substituted 0-4
 carbon atoms with a substituent independently selected
 at each occurrence from the group C₁₋₆ alkyl, C₃₋₆
 25 cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro,
 -OR¹⁷, SH, -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸,
 -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CONR¹⁷R¹⁹, -NR¹⁵CO₂R¹⁸,
 -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and each heteroaryl being
 substituted on any nitrogen atom with 0-1 substituents
 30 selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and
 SO₂R^{14a}.

In another preferred embodiment, R¹ is other than a
 cyclohexyl-(CH₂)_{1, 2, 3, 4, 5, 6, 7, 8, 9, or 10}- group.

35

- In another preferred embodiment, R^1 is other than an aryl-
(CH₂)_{1, 2, 3, 4, 5, 6, 7, 8, 9, or 10}- group, wherein the
aryl group is substituted or unsubstituted.
- 5 In another preferred embodiment, R^1 is other than a
heteroaryl-(CH₂)_{1, 2, 3, 4, 5, 6, 7, 8, 9, or 10}- group,
wherein the heteroaryl group is substituted or
unsubstituted.
- 10 In another preferred embodiment, R^1 is other than a
heterocyclyl-(CH₂)_{1, 2, 3, 4, 5, 6, 7, 8, 9, or 10}- group,
wherein the heterocyclyl group is substituted or
unsubstituted.
- 15 In another preferred embodiment, when D is imidazole or
triazole, R^1 is other than unsubstituted C_{1, 2, 3, 4, 5,}
6, 7, 8, 9, or 10 linear or branched alkyl or
C_{3, 4, 5, 6, 7, or 8} cycloalkyl.
- 20 In another preferred embodiment, R^{1a} is not substituted with
OR¹⁷.

Many compounds of this invention have one or more
25 asymmetric centers or planes. Unless otherwise indicated, all
chiral (enantiomeric and diastereomeric) and racemic forms are
included in the present invention. Many geometric isomers of
olefins, C=N double bonds, and the like can also be present in
the compounds, and all such stable isomers are contemplated in
30 the present invention. The compounds may be isolated in
optically active or racemic forms. It is well known in the art
how to prepare optically active forms, such as by resolution
of racemic forms or by synthesis from optically active
starting materials. All chiral, (enantiomeric and
35 diastereomeric) and racemic forms and all geometric isomeric
forms of a structure are intended, unless the specific
stereochemistry or isomer form is specifically indicated.

The term "alkyl" includes both branched and straight-chain alkyl having the specified number of carbon atoms.

"Alkenyl" includes hydrocarbon chains of either a straight or branched configuration and one or more unsaturated

5 carbon-carbon bonds which may occur in any stable point along the chain, such as ethenyl, propenyl, and the like.

"Alkynyl" includes hydrocarbon chains of either a straight or branched configuration and one or more triple carbon-carbon bonds which may occur in any stable point along the

10 chain, such as ethynyl, propynyl and the like. "Haloalkyl" is intended to include both branched and straight-chain alkyl having the specified number of carbon atoms,

substituted with 1 or more halogen; "alkoxy" represents an alkyl group of indicated number of carbon atoms attached

15 through an oxygen bridge; "cycloalkyl" is intended to include saturated ring groups, including mono-, bi- or polycyclic ring systems, such as cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, and so forth. "Halo" or "halogen" includes fluoro, chloro, bromo, and iodo.

20 The term "substituted", as used herein, means that one or more hydrogen on the designated atom is replaced with a selection from the indicated group, provided that the designated atom's normal valency is not exceeded, and that the substitution results in a stable compound. When a

25 substituent is keto (i.e., =O), then 2 hydrogens on the atom are replaced.

Combinations of substituents and/or variables are permissible only if such combinations result in stable compounds. By "stable compound" or "stable structure" is

30 meant a compound that is sufficiently robust to survive isolation to a useful degree of purity from a reaction mixture, and formulation into an efficacious therapeutic agent.

The term "pharmaceutically acceptable salts" includes

35 acid or base salts of the compounds of formulas (I) and (II). Examples of pharmaceutically acceptable salts include, but are not limited to, mineral or organic acid salts of basic residues such as amines; alkali or organic

salts of acidic residues such as carboxylic acids; and the like.

Pharmaceutically acceptable salts of the compounds of the invention can be prepared by reacting the free acid or
5 base forms of these compounds with a stoichiometric amount of the appropriate base or acid in water or in an organic solvent, or in a mixture of the two; generally, nonaqueous media like ether, ethyl acetate, ethanol, isopropanol, or acetonitrile are preferred. Lists of suitable salts are
10 found in Remington's Pharmaceutical Sciences, 17th ed., Mack Publishing Company, Easton, PA, 1985, p. 1418, the disclosure of which is hereby incorporated by reference.

"Prodrugs" are considered to be any covalently bonded carriers which release the active parent drug of formula
15 (I) or (II) *in vivo* when such prodrug is administered to a mammalian subject. Prodrugs of the compounds of formula (I) and (II) are prepared by modifying functional groups present in the compounds in such a way that the modifications are cleaved, either in routine manipulation
20 or *in vivo*, to the parent compounds. Prodrugs include compounds wherein hydroxy, amine, or sulfhydryl groups are bonded to any group that, when administered to a mammalian subject, cleaves to form a free hydroxyl, amino, or sulfhydryl group, respectively. Examples of prodrugs
25 include, but are not limited to, acetate, formate and benzoate derivatives of alcohol and amine functional groups in the compounds of formulas (I) and (II); and the like.

The term "therapeutically effective amount" of a compound of this invention means an amount effective to
30 antagonize abnormal level of CRF or treat the symptoms of affective disorder, anxiety, depression, immunological, cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathological disturbance and stress in a host.

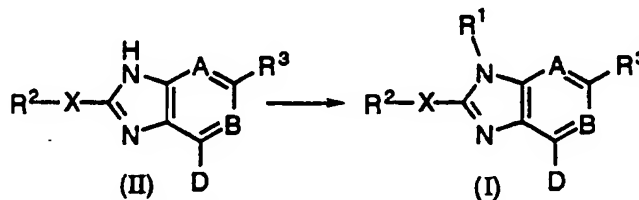
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Synthesis

Compounds of formula (I) can be prepared by the following synthetic routes and schemes. Where a detailed description is not provided, it is assumed that those skilled in the art of organic synthesis will readily understand the meaning.

Synthesis of compounds of formula (I) may be prepared by the reaction shown in Scheme 1.

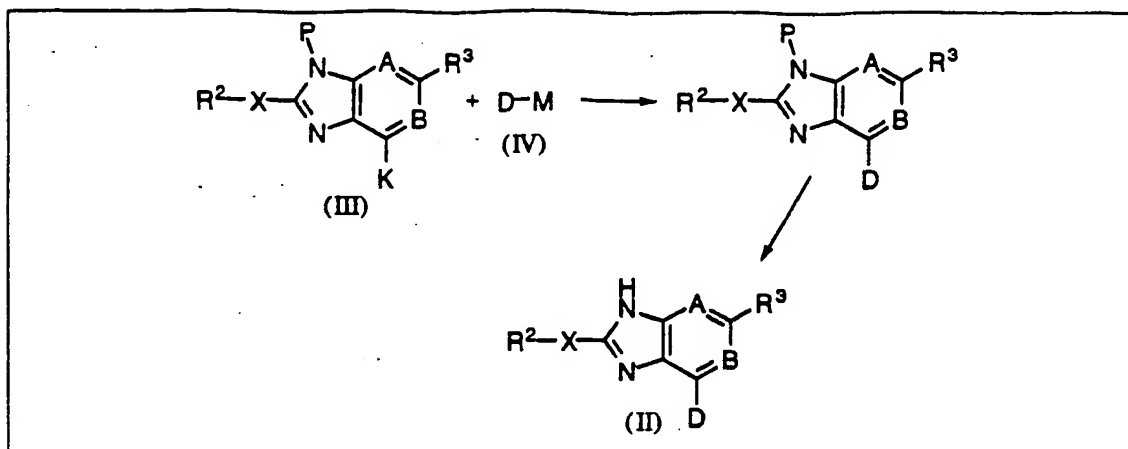
Scheme 1



A compound of formula (II) can be alkylated on the imidazole nitrogen atom with an appropriate reagent. Typical conditions for this transformation include treatment of compound (II) with a base, such as sodium hydride, potassium *tert*-butoxide, sodium hexamethyldisilazide, etc., followed by a reagent J-R¹, where J represents a halide (chloride, bromide or iodide) or pseudohalide (tosylate, mesylate, triflate, etc.), at an appropriate temperature (0 °C or room temperature, with warming if necessary) in a solvent such as tetrahydrofuran, dimethylformamide or dimethylsulfoxide. Alternatively, this reaction may be performed using the Mitsunobu conditions (Mitsunobu, *Synthesis* 1981, pp. 1-28). The compound (II) is treated with an alcohol compound R¹OH, along with a phosphine (triphenyl, tributyl, etc.) and a phosphine-activating reagent such as diethyl azodicarboxylate.

Compounds of Formula (II) may be prepared according to the route shown in Scheme 2.

Scheme 2



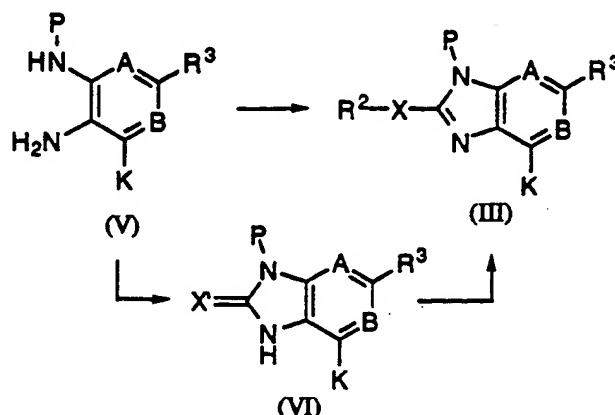
A compound of Formula (III) may be coupled to an aromatic compound of Formula (IV), with elimination of the elements of M-K. For compound (III), K represents a halide, pseudohalide (such as mesylate, tosylate or triflate), or thiomethyl, and P represents a protecting group (if the conditions of the reaction warrant protection of the imidazole N-H; otherwise, P can be H). Suitable P groups may include benzyl, 4-methoxybenzyl, methoxymethyl, trimethylsilylethoxymethyl, *tert*-butoxycarbonyl or benzyloxycarbonyl. For compound (IV), M represents groups such as lithium, bromomagnesium, chlorozinc, (dihydroxy)boron, (dialkoxy)boron, trialkylstannyl and the like. The coupling reaction may be performed in the presence of an appropriate catalyst, such as

tetrakis(triphenylphosphine)palladium, bis(triphenylphosphine)palladium dichloride, [1,3-bis(diphenylphosphino)propane]nickel dichloride, etc. Two particularly useful methods involve the coupling of chloroheterocycles with *in-situ*-prepared arylzinc reagents according to the method of Negishi et al. (*J. Org. Chem.* **1977**, *42*, 1821), and the coupling with arylboronic esters according to the method of Suzuki et al. (*Chem. Letters* **1989**, 1405). Appropriate solvents for reactions of this type usually include tetrahydrofuran, diethyl ether, dimethylformamide, or dimethylsulfoxide. Typical temperatures range from ambient up to the boiling point of the solvent. Once coupled, the P group may be removed to afford compound (II). Conditions for the removal of the protecting groups are well known to those familiar to the art of organic synthesis; e.g. hydrogenation

to remove benzyl or benzyloxycarbonyl, a fluoride source (such as tetrabutylammonium fluoride) to remove silylethoxymethyl, an acid source (such as trifluoroacetic acid) to remove tert-butoxycarbonyl or 4-methoxybenzyl, etc.

- 5 Compounds of formula (III) can be prepared according to the plan shown in Scheme 3.

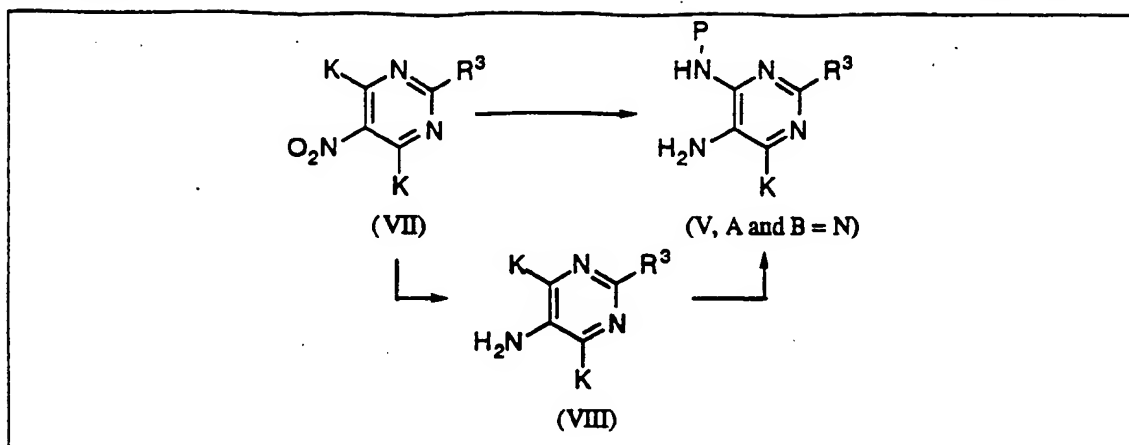
Scheme 3



- 10 A diamine compound of formula (V) (in this case, P is a group such as benzyl, which can be introduced already attached to the nitrogen atom; otherwise, P could represent H initially, and another protecting group being introduced in a later step) is used in a cyclocondensation reaction to make the imidazole ring. The conditions used will, of course, depend on the X
- 15 group chosen, and may include the intermediacy of the compound (VI). A review of imidazole-forming reactions may be found in *Comprehensive Heterocyclic Chemistry* (Pergamon Press, 1984) vol. 5, pp. 457-498.

- 20 Preparation of compounds of formula (V) wherein both A and B are nitrogen atoms may proceed according to the route of Scheme 4.

Scheme 4



A compound of formula (VII) may be available from commercial sources, particularly for K = chloride. Compounds bearing psuedohalide K groups may be available from the corresponding

5 dihydroxy compounds by treatment with an appropriate activating reagent, such as an organosulfonic anhydride or sulfonyl chloride. Compound (VII) may be converted to (V) by either (i) monoalkylation with a compound P-NH₂, followed by reduction of the nitro group; (ii) reduction of the nitro

10 group, to give an amine compound of formula (VIII), followed by monoalkylation with a compound P-NH₂; or (iii) use of a source of ammonia (ammonia gas, ammonium hydroxide, etc.) in either route, followed by protection of the amine group with the group P. Pyrimidine chemistry of this type is well

15 represented in the literature, and is reviewed in *Comprehensive Heterocyclic Chemistry*, vol. 6. Alkylation of chloropyrimidines with amine compounds can be accomplished under either acidic (e.g. HCl or acetic) or basic

(trialkylamines, potassium *tert*-butoxide, etc.) conditions.

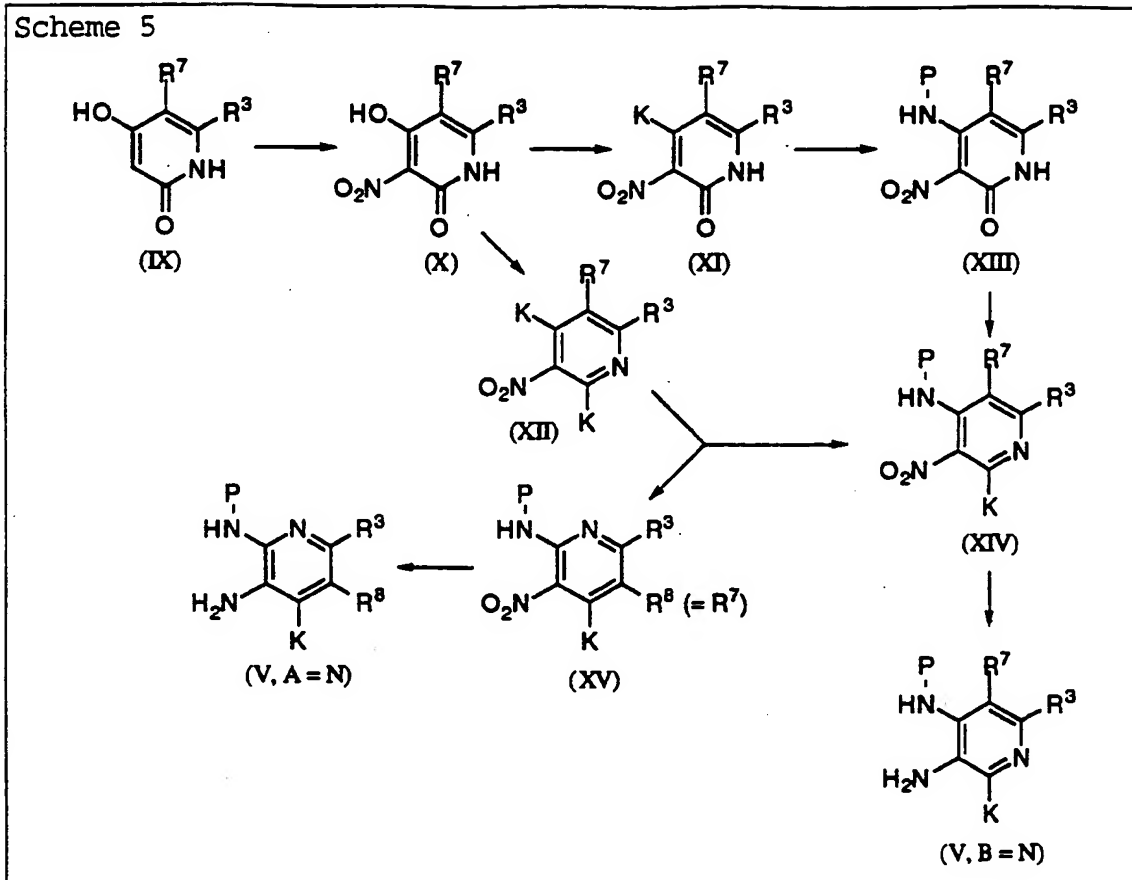
20 Nitro groups in compounds of this type can be reduced to amino groups using one of any number of conditions, including catalytic hydrogenation, tin dichloride, sodium dithionite, zinc metal, iron powder, etc.

Preparation of compounds of formula (V) wherein either A

25 or B represent nitrogen atoms is shown in Scheme 5.

5

Scheme 5

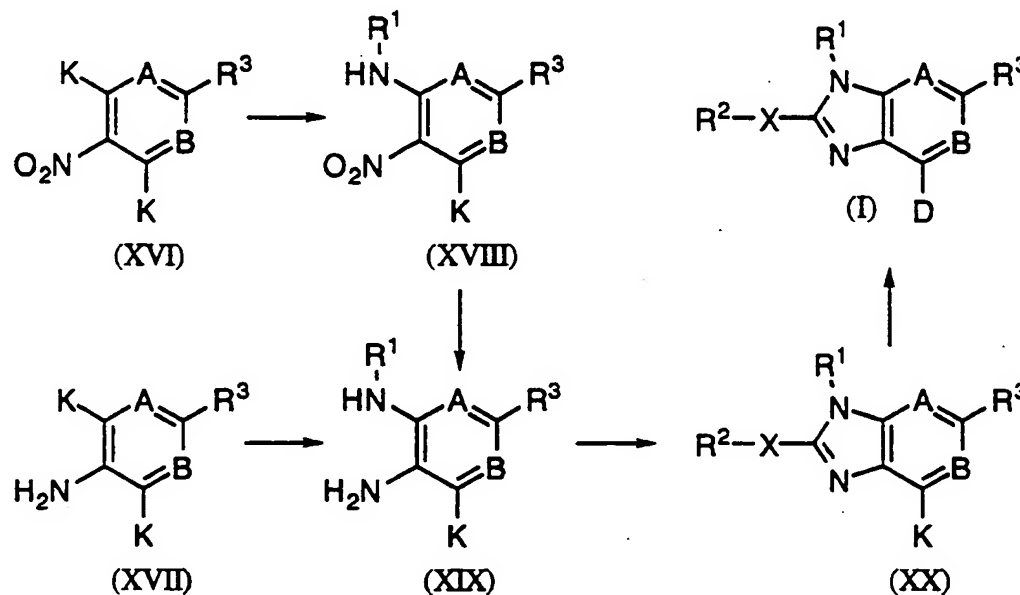


- An hydroxypyridone compound of formula (IX) can be nitrated to give compound (X) employing conditions such as concentrated or fuming nitric acid, optionally in the presence of concentrated sulfuric or acetic acid. The hydroxypyridone can be selectively monoactivated with a K group to give a compound of formula (XI); one method to do this involves treatment of the dicyclohexylamine salt of compound (X) with phosphorus oxychloride to give (XI) wherein K = Cl. Alternatively, both the hydroxy and pyridone groups in compound (X) can be activated at the same time, using stronger conditions such as phosphorus oxychloride and heat, or excess toluenesulfonic anhydride, to give compound (XII). Compound (XI) may be converted to the protected amine compound (XIII) using the same general route discussed above for the pyrimidines.

Selective monoalkylation using compound (XII) is also possible, but will probably give mixtures of regioisomeric products (XIV) and (XV). The nitro groups in these compounds can then be reduced as discussed above, to give compounds for
 5 formula (V) wherein either A or B is nitrogen.

An alternative approach to the method involving introduction of the R^1 group at the initial step is shown in Scheme 6.

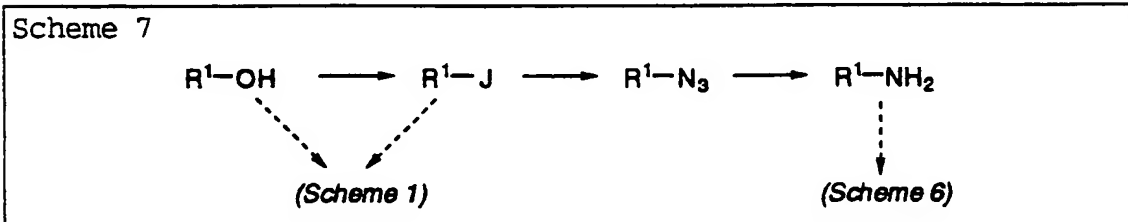
Scheme 6



This is particularly useful in the cases where R^1 represents a group where alkylation of compound (II) is impractical (e.g. a very bulky R^1 group), but can also be used in a general manner. Here, compounds of formula (XVI) or (XVII)
 15 (either amino- or nitro-pyridines or pyrimidines) are alkylated with an amine reagent R^1 -NH₂, under either acidic or basic conditions as described above. Nitro compound (XVIII) can be converted to amine compound (XIX) by nitro reduction reactions described earlier. Compound (XIX) can
 20 be cyclized to imidazole compound (XX). As above, this reaction will depend upon the choice of X group. For example, for $X = CHR^9$, one can use an orthoester reagent such as $R^2CH(R^9)C(OR)_3$, with heating in neat solution or high-boiling solvents, and the optional presence of an acid
 25 catalyst (such as hydrochloric or sulfuric acid) (see

Montgomery and Temple, *J. Org. Chem.* **1960**, *25*, 395). For $X = NR^{10}$, the cyclization is performed using reagents such as an guanidine reagent of the structure $R^2R^{10}N-C(=NH)NH_2$ or a urea-derived reagent of the structure $R^2R^{10}N-C(=NH)D$, where D represents a group like OCH_3 , SCH_3 or SO_2CH_3 . For $X = O$, the ring is formed using a reagent of the structure $(R^2O)_4C$ (with acetic acid catalysis), provided one has access to the reagent with the R^2 group of choice (see Brown and Lynn, *J. Chem. Soc. Perkin Trans. I* **1974**, 349). Alternatively, the diamine (XIX) is treated with phosgene, followed by O-alkylation to introduce the R^2 group (such as a reagent like R^2-I or R^2-Br). A similar route can be used for $X = S$, which would use thiophosgene or some similar reagent, followed by S-alkylation with the R^2 group. The sulfur atom in this compound (and sulfide groups throughout the molecule in general) can be oxidized to either the sulfoxide or sulfone if desired by treatment with an appropriate oxidizing agent such as potassium permanganate, potassium peroxomonosulfate or m-chloroperbenzoic acid. Finally, compound (XX) can be used in an aryl coupling reaction as described above to replace the K group with the desired aryl group in compound (I).

Methods of synthesis of compounds R^1-OH , R^1-J and R^1-NH_2 are related, in that the alcohol can be used in the synthesis of the other two compounds, as is shown in Scheme 7.

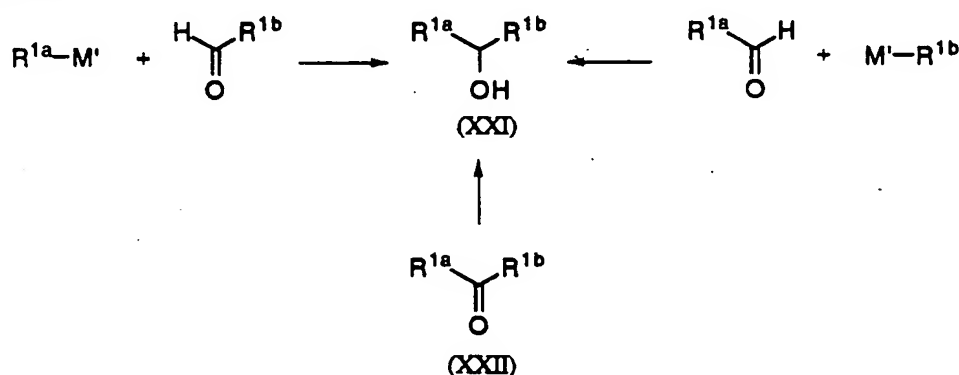


For example, the hydroxy group may be converted to the following J groups, using the indicated reagents (this route is not limited to these J groups): methanesulfonate, using methanesulfonyl chloride or anhydride and an appropriate base; toluenesulfonate, using toluenesulfonyl chloride or anhydride and an appropriate base; iodide; using iodine / triphenylphosphine; bromide, using phosphorus tribromide or

carbon tetrabromide / triphenylphosphine; or trifluoromethanesulfonate, using trifluoromethane-sulfonic anhydride and an appropriate base. Both compounds $R^1\text{-OH}$ and $R^1\text{-J}$ are used in the methods portrayed in Scheme 1. Conversion of $R^1\text{-J}$ to $R^1\text{-N}_3$ requires the use of an azide source, such as sodium azide, and a solvent such as dimethylsulfoxide or dimethylformamide, or water and a phase-transfer catalyst (such as tetrabutylammonium hydrogen sulfate). Reduction of the azide compound $R^1\text{-N}_3$ to $R^1\text{-NH}_2$ may be accomplished using reagents such as sodium borohydride or triphenylphosphine, or hydrogen gas and a catalyst (such as palladium on carbon). The amine $R^1\text{-NH}_2$ may then be employed in the methods portrayed in Scheme 6.

In the cases where the compound $R^1\text{-OH}$ could be represented by a structure of formula (XXI) (Scheme 8), wherein R^{1a} and R^{1b} represents substructures which, taken together with the carbinol methine group, comprise the entire group R^1 , this compound may be prepared by addition to a carbonyl compound.

Scheme 8

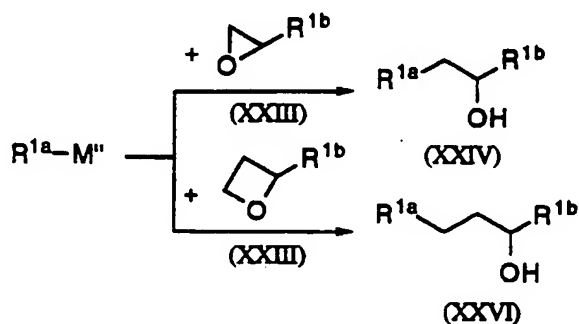


This route is particularly useful in the case where R^{1a} or R^{1b} represents a cycloalkyl group, such as cyclopropyl. An organometallic reagent (where M' represents a metallic group, such as Li, CuCN, CuI, MgCl, MgBr, MgI, ZnCl, CrCl, etc.) can be allowed to react with an aldehyde reagent to prepare the alcohol compound of formula (XXI). Alternatively, a ketone of formula (XXII) may be treated with a reducing agent, such as sodium borohydride, lithium aluminum hydride, etc., which will

also generate the alcohol of formula (XXI). Standard methods of ketone synthesis may be used where appropriate in the preparation of compounds for formula (XXII), which will be familiar to those skilled in the art of organic synthesis.

- 5 An homologous approach may also be employed in the synthesis of alcohols $R^1\text{-OH}$, involving the ring-opening reaction of cyclic ether compounds with organometallic reagents (Scheme 9).

10 Scheme 9

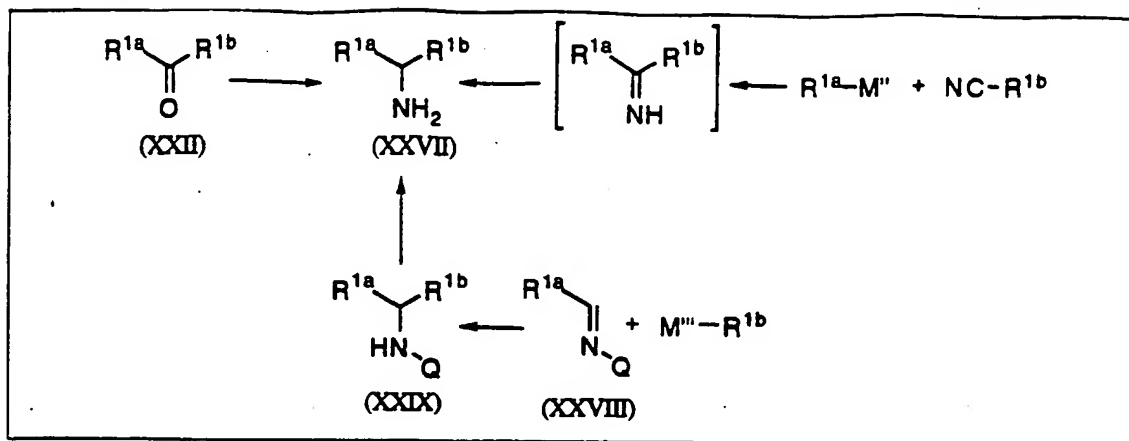


- Here, an organometallic reagent $R^{1a}\text{-M}''$ is used, where M'' represents metals such as Mg, Zn or Cu. Especially useful is the method described in Huynh, et al., Tetrahedron Letters 1979, (17), pp. 1503-1506, where organomagnesium reagents are allowed to react with cyclic ethers with catalysis provided by copper (I) iodide. Use of an epoxide compound of formula (XXIII) in this manner would result in synthesis of an alcohol compound of formula (XXIV), and use of an oxetane compound of formula (XXV) would generate an alcohol of formula (XXVI). Both compounds (XXIV) and (XXVI) are variants of $R^1\text{-OH}$.

Synthesis of compound $R^1\text{-NH}_2$ with formula (XXVII) is portrayed in Scheme 10.

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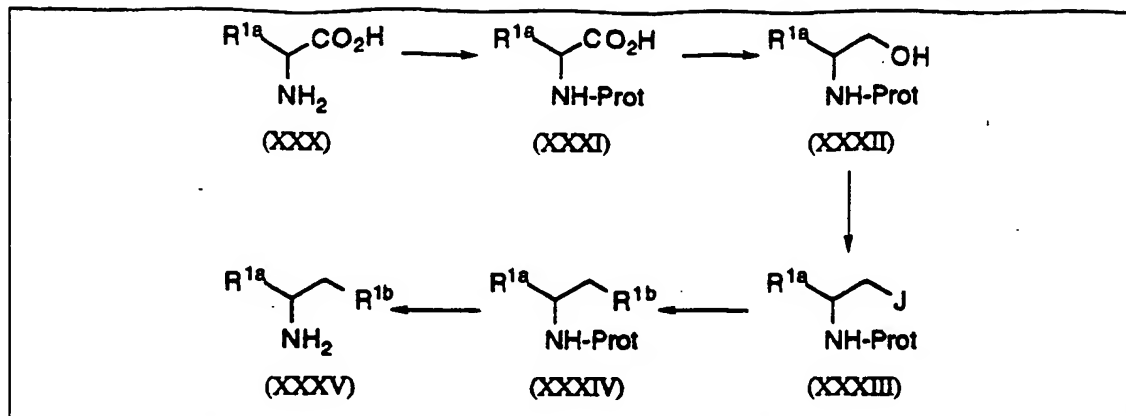
Scheme 10



A simple reductive amination of ketone (XXII) will produce
 5 amine (XXVII). This reaction may be performed using anhydrous
 ammonia in the presence of hydrogen and a catalyst.
 Alternatively, addition of an organometallic reagent to a
 nitrile compound gives an imine, which may be treated in situ
 with a reducing agent (such as sodium cyanoborohydride) to
 10 give amine (XXVII). Finally, a compound of formula (XXVIII),
 wherein Q is an optionally-substituted oxygen atom (i.e. an
 oxime) or nitrogen atom (i.e. a hydrazone), may be allowed to
 react with an organometallic reagent $R^{1b}-M'''$. Here, metallic
 groups M''' such as MgBr, CuCl or CeCl₂ have been used in
 15 additions to oximes or hydrazones. The intermediate addition
 products of formula (XXIX) may be subjected to reductive
 cleavage (using conditions such as sodium/liquid ammonia or
 catalytic hydrogenation), which will afford amines (XXVII).

Amino acids, either naturally-occurring or synthetic, are
 20 potential sources of useful starting materials for the
 synthesis of the compounds of this invention. Scheme 11 shows
 some possible applications of this approach.

Scheme 11



Protected amino acids of formula (XXXI) are prepared from the parent compounds of formula (XXX); useful protecting groups ("Prot") include tert-butoxycarbonyl, benzyloxycarbonyl and triphenylmethyl. Standard texts in peptide chemistry describe this protection. The carboxylic acid group may be reduced using reagents such as lithium borohydride, which gives alcohol (XXXII). The hydroxy group may be converted to a leaving group "J" as described before. The compound of formula (XXXIII) may be treated with appropriate reagents to produce a wide variety of functional groups included in the scope of this invention (compound (XXXIV)); displacement of J with cyanide (sodium cyanide in warm dimethylformamide may be used here) gives a nitrile, displacement of J with a mercaptan (in the presence of a base, such as potassium carbonate) gives a disulfide, displacement of J with a secondary amine gives a tertiary amine, etc.

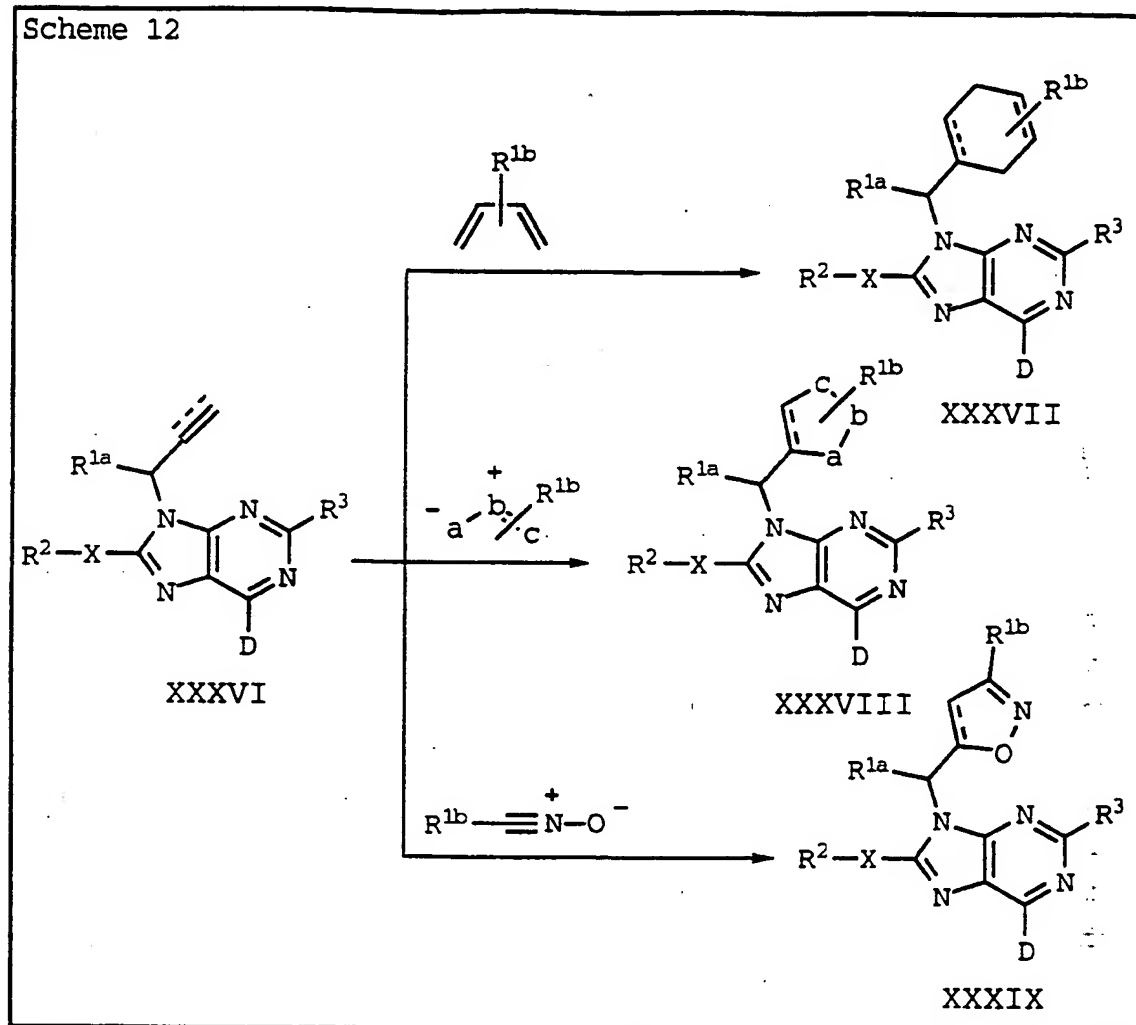
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The compounds of Formula (I) with unsaturated R¹ groups can be a further source of compounds covered under this invention. Unsaturated (double and triple) bonds can take part in cycloaddition chemistry with appropriate reagents (Scheme 12). Cycloaddition of an alkyne compound of Formula XXXVI with 1,3-dienes to give six-membered ring compounds like that of Formula XXXVII (commonly known as the Diels-Alder reaction), and cycloaddition with 3-atom dipolar reagents to give heterocyclic compounds of Formula XXXVIII, are familiar to those skilled in the art of organic synthesis. One specific

30

example of this approach is the synthesis of an isoxazole compounds of Formula XXXIX from the alkyne XXXVI and a nitrile oxide reagent.

5 Scheme 12

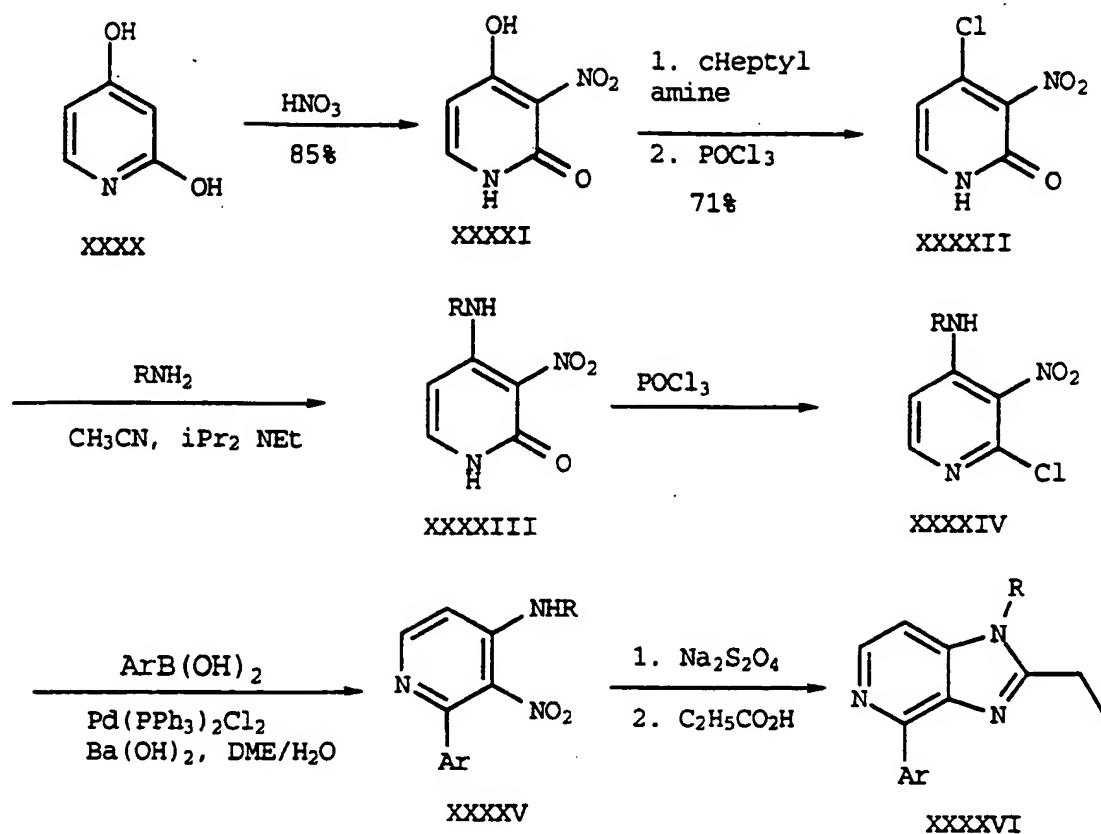


10 The synthetic procedure in Scheme 13 shown below may be used to prepare 4,5-c imidazopyridines.

15

20

Scheme 13



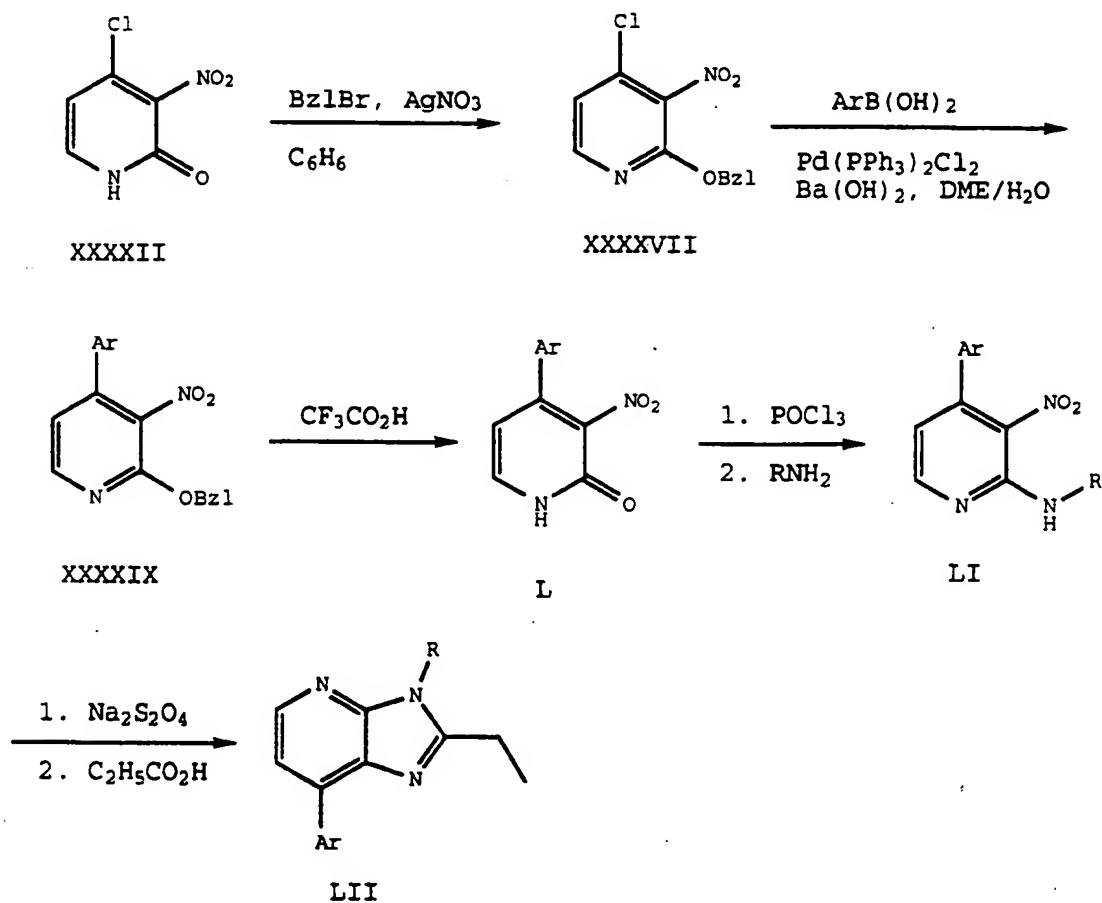
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- 10 Nitration of 2,4-dihydroxypyridine (XXXX) with HNO_3 as described earlier (Koagel et al. Recl. Trav. Chim. Pays-Bas. 29, 38, 67, 1948) gave the corresponding 3-nitropyridone (XXXXXI) which was treated with an organic amine base, such as cycloheptyl amine to give selectively the corresponding 4-
- 15 chloropyridone (XXXXXII). This in turn was reacted with a primary amine RNH_2 , where R is a group described earlier in an aprotic or protic solvent, such as CH_3CN , DMSO, DMF, or an alkyl alcohol in the presence of an organic or inorganic base, such as a trialkylamine, K_2CO_3 , Na_2CO_3 etc, and in temperature
- 20 range of 20-200 °C to give the 4-amino adduct (XXXXXIII). Pyridone (XXXXXIII) was converted to the 2-chloropyridine (XXXXXIV) by treatment with POCl_3 , and (XXXXXIV) was coupled with an arylboronic acid ArB(OH)_2 under palladium catalysis to

give (XXXXV). Nitropyridine (XXXXV) was reduced to the corresponding aminopyridine by use of $\text{Na}_2\text{S}_2\text{O}_4$ or a Fe, Sn or SnCl_2 , and converted to the imidazo[4,5-c]pyridine in refluxing propionic acid. The same transformation can be affected by the use of a nitrile, an imidate, thioimide or trialkylorthopropionate.

The synthetic procedure in Scheme 14 shown below may be used to prepare 4,5-b imidazopyridines.

Scheme 14



20

Reaction of 4-chloropyridone (XXXXII) with an aryl halide, such as benzyl bromide in benzene and in the presence of Ag_2CO_3 as described in Scheme 13 (Smith A. M.; et al. J. Med. Chem. 36, 8, 1993) and at temperature ranges of 30-80 °C afforded the corresponding 2-benzyloxypyridine (XXXXVII). This was coupled with an arylboronic acid, $\text{ArB}(\text{OH})_2$, under palladium-catalyzed conditions to give (XXXXIX). The benzyloxy group can be removed by treatment with a strong acid, such as trifluoroacetic, triflic, sulfuric, HCl , etc. to give pyridone (L). This was converted to the 2-halopyridine with the action of POX_3 , PX_5 or the corresponding triflate, tosylate or mesylate, which was displaced with a primary amine RNH_2 to give (LI). The nitro group was reduced under conditions described in scheme 13 and the aminopyridine was cyclized to the imidazolo[4,5-b]pyridine (LII) under conditions described in scheme 13.

The following examples are provided to describe the invention in further detail. These examples, which set forth the best mode presently contemplated for carrying out the invention, are intended to illustrate and not to limit the invention.

The methods discussed below in the preparation of 8-ethyl-9-(1-ethylpentyl)-6-(2,4,6-trimethylphenyl)purine (Table 1, Example 2, Structure A) and 9-butyl-8-ethyl-6-(2,4,6-trimethylphenyl)purine (Table 1, Example 27, Structure A) may be used to prepare all of the examples of Structure A contained in Table 1, Table 1A and Table 1B, with minor procedural modifications where necessary and use of reagents of the appropriate structure.

The methods discussed below in the preparation of 3-(1-cyclopropylpropyl)-7-(2,4-dichlorophenyl)-2-ethyl-3H-imidazo[4,5-b]pyridine (Table 1, Example 38, Structure B) and 1-(1-cyclopropylpropyl)-4-(2,4-dichlorophenyl)-2-ethyl-1H-imidazo[4,5-c]pyridine (Table 1, Example 38, Structure C) may be used to prepare many of the examples of

- Structures B and C contained in Table 1, Table 1A, Table 1B and Table 1C, with minor procedural modifications where necessary and use of reagents of the appropriate structure.

5

Example 2

Preparation of 8-Ethyl-9-(1-ethylpentyl)-6-(2,4,6-trimethylphenyl)purine

- 10 Part A. A solution of 5-amino-4,6-dichloropyrimidine (10.0 g, 61.0 mmol) and triethylamine (12.8 mL, 91.5 mmol) in ethanol (100 mL) was treated with benzylamine (7.30 mL, 67.1 mmol), and heated to 50 °C overnight. The resulting mixture was cooled, and the resulting crystalline solid was collected by
15 filtration. The solid was triturated with hexane, refiltered and dried under vacuum. A second crop was collected from the mother liquor and purified like the first crop to afford in total 12.67 g (48.8 mmol, 80%) of 5-amino-6-benzylamino-4-chloropyrimidine. TLC R_f 0.10 (30:70 ethyl acetate-hexane). ^1H
20 NMR (300 MHz, CDCl_3): δ 7.62 (1H, s), 7.13-6.97 (5H, m), 6.61 (1H, br t, J = 5 Hz), 4.43 (2H, d, J = 5.5 Hz), 4.24 (2H, br s). MS ($\text{NH}_3\text{-CI}$): m/e 238 (4), 237 (33), 236 (15), 235 (100).

- Part B. A solution of the diamine from Part A (10.45 g, 44.5
25 mmol) and 3 drops concentrated hydrochloric acid in triethyl orthopropionate (70 mL) was heated to 100 °C for 1 hour, then cooled, poured into water (200 mL) and extracted with ethyl acetate (2 x 200 mL). The extracts were washed in sequence with brine (100 mL), then combined, dried over anhydrous
30 sodium sulfate, filtered and evaporated. The residue was separated by column chromatography (silica gel, 20:80 ethyl acetate-hexane) to afford the product, N-(6-benzylamino-4-chloropyrimidin-5-yl)-O-ethyl-propionimide (12.82 g, 40.2 mmol, 90%) as a crystalline solid, m.p. 85-86 °C. TLC R_f 0.25
35 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.19 (1H, s), 7.35-7.29 (5H, m), 5.21 (1H, br t, J = 5 Hz), 4.70 (2H, d, J = 5.9 Hz), 4.29 (2H, br), 2.15 (2H, br q, J = 7.3

Hz), 1.35 (3H, t, $J = 7.0$ Hz), 1.06 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 322 (6), 321 (34), 320 (20), 319 (100).

Part C. A solution of the imidate compound prepared in Part B
5 above (10.66 g, 33.4 mmol) and p-toluenesulfonic acid monohydrate (100 mg) in diphenyl ether (10 mL) was heated to 170 °C for 2 hours. The resulting mixture was cooled and poured into 50 mL water. This was extracted with ethyl acetate (2 x 50 mL), and the extracts were washed in sequence with
10 brine (50 mL), combined, dried over anhydrous sodium sulfate, filtered and evaporated. The residual material was separated by column chromatography (silica gel, hexane to remove diphenyl ether, then 30:70 ethyl acetate-hexane) to afford the product, 9-benzyl-6-chloro-8-ethylpurine, as an oil (8.16 g,
15 29.9 mmol, 89%). TLC R_f 0.20 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): d 8.72 (1H, s), 7.37-7.29 (3H, m), 7.19-7.14 (2H, m), 5.46 (2H, s), 2.89 (2H, q, $J = 7.7$ Hz), 1.38 (3H, t, $J = 7.7$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 276 (6), 275 (36), 274 (20), 273 (100).

20

Part D. A solution of zinc chloride (5.32 g, 39.1 mmol) in anhydrous, freshly-distilled tetrahydrofuran (50 mL) was treated at ambient temperature with a solution of mesitylmagnesium bromide (39.1 mL, 1.0 M, 39.1 mmol) in
25 diethyl ether. After 45 minutes, a separate flask containing a solution of bis(triphenylphosphine)-palladium dichloride (0.92 g, 1.3 mmol) in tetrahydrofuran (30 mL) was treated with a solution of diisobutylaluminum hydride (2.6 mL, 1.0 M, 2.6 mmol) in hexane. This mixture was allowed to stir for 15
30 minutes, then treated with the mesitylzinc chloride solution dropwise by cannula. Then, the chloropurine compound in 10 mL tetrahydrofuran solution was added by syringe, and the mixture was allowed to stir for 12 hours at ambient temperature. It was poured into water (150 mL), and acidified with dropwise
35 addition of 1 N aqueous hydrochloric acid until the mixture is homogeneous. This is extracted with ethyl acetate (2 x 150 mL), and the extracts were washed in sequence with saturated brine solution (100 mL), combined, dried over anhydrous sodium

sulfate, filtered and evaporated. The residue was separated by column chromatography (silica gel, 30:70 ethyl acetate-hexane) to afford the product, 9-benzyl-8-ethyl-6-(2,4,6-trimethylphenyl)purine (6.68 g, 18.7 mmol, 72%), as an off-white waxy solid, m.p. 121-122 °C. ¹H NMR (300 MHz, CDCl₃): δ 9.00 (1H, s), 7.38-7.31 (3H, m), 7.23-7.21 (2H, m), 6.96 (2H, s), 5.50 (2H, s), 2.84 (2H, q, J = 7.6 Hz), 2.33 (3H, s), 2.06 (6H, s), 1.26 (3H, t, J = 7.5 Hz). MS (NH₃-CI): m/e 359 (3), 358 (26), 357 (100).

10

Part E. A solution of the benzyl compound from Part D above (5.33 g, 14.95 mmol) in trifluoroacetic acid (320 mL) partitioned into four Parr bottles, and each was treated with 0.8 g 20% palladium hydroxide on carbon. The bottles were each subjected to hydrogenation (50 psi) in shaker apparatus for 18 hours. The atmospheres were purged with nitrogen, and the solutions were combined, filtered through celite and evaporated. The residual material was separated by column chromatography (silica gel, 50:50 ethyl acetate-hexane) to afford the product, 8-ethyl-6-(2,4,6-trimethylphenyl)purine (3.75 g, 14.1 mmol, 94%), as a white crystalline solid, m.p. 215-217 °C. TLC R_f 0.17 (50:50 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 12.35 (1H, br s), 9.03 (1H, s), 6.96 (2H, s), 3.05 (2H, q, J = 7.7 Hz), 2.32 (3H, s), 2.05 (6H, s), 1.50 (3H, t, J = 7.7 Hz). MS (NH₃-CI): m/e 269 (2), 268 (19), 267 (100).

Part F. A solution of the purine compound from Part E above (200 mg, 0.75 mmol), 3-heptanol (0.13 mL, 0.90 mmol) and triphenylphosphine (0.24 g, 0.90 mmol) in freshly-distilled tetrahydrofuran (5 mL) was cooled to 0 °C, and treated with diethyl azodicarboxylate (0.14 mL, 0.90 mmol) dropwise by syringe. The mixture was allowed to stir for 12 hours, then evaporated. The residual material was separated by column chromatography (silica gel, 15:85 ethyl acetate-hexane) to afford the title product as a white solid (0.152 g, 0.42 mmol, 56%), m.p. 99-100 °C. TLC R_f 0.17 (10:90 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.91 (1H, s), 6.95 (2H, s),

4.22 (1H, br), 2.92 (2H, q, $J = 7.7$ Hz), 2.41 (2H, br), 2.32 (3H, s), 2.10-1.98 (2H, m), 2.05 (3H, s), 2.04 (3H, s), 1.37 (3H, t, $J = 7.5$ Hz), 1.34-1.23 (4H, m), 0.84 (3H, t, $J = 7.1$ Hz), 0.81 (3H, t, $J = 7.5$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 367 (3), 366 (27), 365 (100).

Example 27

Preparation of 9-Butyl-8-ethyl-6-(2,4,6-trimethylphenyl)purine

10 A solution of 8-ethyl-6-(2,4,6-trimethylphenyl)purine (200 mg, 0.75 mmol) in anhydrous dimethylformamide (5 mL) was cooled to 0 °C, and treated with sodium hydride dispersion in mineral oil (72 mg 50% w/w, 1.50 mmol). After 1 hour, bromobutane (0.10 mL, 0.90 mmol) was added by syringe, and the mixture was
15 allowed to stir for 12 hours. It was poured into ethyl acetate (120 mL), and was washed with water (3 x 120 mL) and brine (100 mL). The aqueous layers were back-extracted in sequence with ethyl acetate (120 mL), and the extracts were combined, dried over anhydrous sodium sulfate, filtered and evaporated.
20 The residue was separated by column chromatography (silica gel, 20:80 ethyl acetate-hexane) to afford the title product as a viscous oil (64.2 mg, 0.20 mmol, 27%). TLC R_f 0.20 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.96 (1H, s), 6.95 (2H, s), 4.25 (2H, t, $J = 7.5$ Hz), 2.93 (2H, q, $J = 7.7$
25 Hz), 2.32 (3H, s), 2.04 (6H, s), 1.91-1.86 (2H, m), 1.50-1.38 (2H, m), 1.39 (3H, t, $J = 7.7$ Hz), 1.01 (3H, t, $J = 7.5$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 325 (3), 324 (23), 323 (100).

Example 35

30 Preparation of 6-(2,4-Dichlorophenyl)-8-ethyl-9-(1-ethylpentyl)purine

A solution of 2,4-dichlorobenzeneboronic acid (572 mg, 3.00 mmol) and ethylene glycol (205 mg, 3.30 mmol) in benzene (20
35 mL) was heated to reflux with azeotropic removal of water for a period of 8 h. The resulting solution was cooled, and treated with 6-chloro-8-ethyl-9-(1-ethylpentyl)purine (see Example 2, Part C above; 562 mg, 2.00 mmol), thallium

carbonate (1.03 g, 2.20 mmol) and
tetrakis(triphenylphosphine)palladium (116 mg, 0.10 mmol). The
resulting mixture was heated to reflux with stirring for 12 h,
then cooled, filtered through celite and evaporated. The
5 resulting residue was separated by column chromatography
(silica gel, 10:90 ethyl acetate-hexane) to afford the title
compound as a viscous oil (530 mg, 1.35 mmol, 68%). TLC R_f
0.31 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ
8.94 (1H, s), 7.71 (1H, d, $J = 8.4$ Hz), 7.58 (1H, d, $J = 1.8$
10 Hz), 7.41 (1H, dd, $J = 8.4, 1.8$ Hz), 4.27 (1H, br), 2.95 (2H,
q, $J = 7.3$ Hz), 2.41 (2H, br), 2.11-1.98 (2H, br), 1.42 (3H,
t, $J = 7.3$ Hz), 1.37-1.20 (3H, m), 1.09-0.99 (1H, m), 0.84
(3H, t, $J = 7.7$ Hz), 0.82 (3H, t, $J = 7.7$ Hz). MS (NH_3 -CI):
 m/e calc'd for $\text{C}_{20}\text{H}_{25}\text{N}_4\text{Cl}_2$: 391.1456, found 391.1458; 395 (11),
15 394 (14), 393 (71), 392 (29), 391 (100).

Example 38

20 Preparation of 3-(1-cyclopropylpropyl)-7-(2,4-dichlorophenyl)-
2-ethyl-3H-imidazo[4,5-b]pyridine

Part A. 2,4-Dihydroxypyridine (15.0 g, 135 mmol) was heated in
 HNO_3 (85 mL) at 80 °C for 15-20 min at which time it went into
solution. The temperature was maintained for 5 min and after
25 cooling it was poured into ice/water (~200 mL). The
precipitated solid was collected and dried (19.0 g, 90%
yield). ^1H NMR (300 MHz, $\text{dmso}-d_6$): 12.3-12.5 (1H, brs), 11.75-
11.95 (1H, brs), 7.41 (1H, d $J = 7.3$ Hz), 5.99 (1H, d $J = 7.3$
30 Hz).

Part B. 4-Hydroxy-3-nitropyridone (8.0 g, 51.25 mmol) and
cycloheptyl amine (6.8 mL, 53.4 mmol) were heated at reflux in
methanol (100 mL) for 15 min. The solvent was stripped off and
the residual solid was washed with 1:1 EtOAc /hexanes and
35 dried under vacuum. The cycloheptyl amine salt was stirred in
 POCl_3 (60 mL) for 40 h and poured into ice/water (~600 mL).
The precipitated product was collected and dried under vacuum

(7.0 g, 78% yield). ^1H NMR(300 MHz, dms O d_6): 12.8-13.05 (1H, brs), 7.73 (1h, d J = 7.0 Hz), 6.50 (1H, d J = 7.0 Hz).

Part C. 4-Chloro-3-nitro-pyridone (0.5 g, 2.86 mmol) Ag_2CO_3 (0.83 g, 3 mmol) and benzyl bromide (0.36 mL, 3 mmol) were stirred in dry benzene (20 mL) at 60 $^\circ\text{C}$ for 5 h. The reaction mixture was filtered and stripped in vacuo. The residue was chromatographed on silica gel (10% EtOAc/hexanes eluent) to give the product (0.6 g, 79%). ^1H NMR(300 MHz, CDCl_3): 8.15 (1 H, d J = 4.0 Hz), 7.30-7.42 (5 H, m), 7.04 (1H, d J = 4.0 Hz), 5.50 (2H, s).

Part D. 2-Benzyloxy-4-chloro-3-nitropyridine (0.5 g, 1.9 mmol), 2,4-dichlorophenylboronic acid (0.363 g, 1.9 mmol) $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (76 mg, 0.11 mmol) and $\text{Ba}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ (0.6 g, 1.9 mmol) were heated at reflux in 1,2-dimethoxyethane (6 mL), and water (6 mL) for 5 h. The mixture was partitioned between EtOAc (100 mL) and water (30 mL) and the EtOAc was washed with water, brine, dried and stripped in vacuo. The residue was chromatographed on silica gel (10% EtOAc/hexanes eluent) to give the product (370 mg, 52% yield). ^1H NMR(300 MHz, CDCl_3): 8.31 (1H, d J = 5.1 Hz), 7.51 (1H, d J = 2.2 Hz), 7.30-7.43 (6 H, m), 7.20 (1H, d J = 8.0 Hz), 6.91 (1H, d J = 5.1 Hz), 5.56 (2h, s).

Part E. 2-Benzyloxy-4-(2,4-dichlorophenyl)-3-nitropyridine (1.65 g, 4.39 mmol) was stirred in $\text{CF}_3\text{CO}_2\text{H}$ (5 mL) at 25 $^\circ\text{C}$ for 4 h. The $\text{CF}_3\text{CO}_2\text{H}$ was stripped in vacuo and the residue was washed with 20% EtOAc/hexanes and used in the next reaction. ^1H NMR(300 MHz, CDCl_3): 7.62 (1H, d J = 7.0 Hz), 7.53 (1H, d J = 2.2 Hz), 7.34 (1H, dd J = 7.0, 2.2 Hz), 7.22 (1H, d J = 8.1 Hz), 6.33 (1H, d J = 7.0 Hz).

Part F. 4-(2,4-dichlorophenyl)-3-nitropyridone (4.39 mmol) was heated at reflux in POCl_3 (5 mL) for 5 h. After cooling it was poured into ice/water (~60 mL) and extracted with EtOAc (2x100 mL). The EtOAc was washed with satNaHCO $_3$, brine, dried and stripped in vacuo. Used in the next reaction without

further purification. ^1H NMR(300 MHz, CDCl_3): 8.60 (1H, d J = 5.2 Hz), 7.54 (1H, d, J = 2.2 Hz), 7.36 (1H, dd J = 8.1, 2.2 Hz), 7.20 (1H, d J = 8.1 Hz).

- 5 Part G. 2-Chloro-4-(2,4-dichlorophenyl)-3-nitropyridine (0.5 g, 1.65 mmol) 1-cyclopropylpropylamine hydrochloride (461 mg, 3.4 mmol) and diisopropyl ethylamine (1.26 mL, 0.72 mmol) were heated at reflux in CH_3CN (10 mL) for 64 h. The mixture was partitioned between EtOAc (70 mL) and water (40 mL). The
10 aqueous layer was extracted with EtOAc (50 mL) and the combined EtOAc extracts washed with brine, dried and stripped in vacuo. The residue was chromatographed on silica gel (10% EtOAc/hexanes eluent) to give the product (310 mg, 51% yield). ^1H NMR(300 MHz, CDCl_3): 8.29 (1H, d J = 4.7 Hz), 7.76 (1H, brd J = 8.0 Hz), 7.46 (1H, d J = 2.2 Hz), 7.32 (1H, dd J = 8.5,
15 2.2 Hz), 7.15 (1H, d J = 8.5 Hz), 3.72-3.85 (1H, m), 1.70-1.80 (2H, m), 0.90-1.08 (4H, m), 0.30-0.66 (4H, m).

- Part H. 2-(1-cyclopropyl)propylamino-4-(2,4-dichlorophenyl)-3-nitropyridine (310 mg, 0.85 mmol) was dissolved in dioxane (8
20 mL) and water (8 mL) containing conc NH_4OH (0.3 mL) was added, followed by $\text{Na}_2\text{S}_2\text{O}_4$ (1.1 g, 6.86 mmol). The reaction was stirred at 25 °C for 4 h and extracted with EtOAc (100 mL). The EtOAc was washed with brine, dried and stripped in vacuo.
25 The residue was chromatographed on silica gel (25% EtOAc/hexanes and ~1% conc NH_4OH eluent) to give the product (150 mg, 53% yield). ^1H NMR(300 MHz, CDCl_3): 7.73 (1H, d J = 5.5 Hz), 7.53 (1H, d J = 1.8 Hz), 7.35 (1H, dd J = 8.1, 1.8 Hz), 7.24 (1H, d J = 8.1 Hz), 6.35 (1H, d J = 5.5 Hz), 4.3
30 (1H, brs), 3.5 (1H, brs), 3.42-3.55 (1H, m), 3.04 (2H, brs), 1.70-1.81 (2H, m), 0.88-1.08 (4H, m), 0.3-0.6 (4H, m).

- Part I. 3-amino-2-(1-cyclopropyl)propylamino-4-(2,4-dichlorophenyl)-pyridine (140 mg, 0.42 mmol) was heated at
35 reflux in propionic acid (5 mL) for 23 h. Then the mixture was diluted with water (50 mL), neutralized with solid NaHCO_3 and basified with 50%NaOH. Then it was extracted with EtOAc (80 mL) and the EtOAc was dried and stripped in vacuo. The

residue was chromatographed on silica gel (10% and 20%EtOAc/hexanes eluant) to give the product, which was crystallized from hexanes (70 mg, 45% yield) mp 118-119 °C. ¹H NMR(300 MHz, CDCl₃): 8.31 (1H, d J = 4.7 Hz), 7.62 (1H, d J = 7.2 Hz), 7.55 (1H, d J = 1.8 Hz), 7.37 (1H, dd J = 7.2, 1.8 Hz), 7.23 (1H, d J = 4.7 Hz), 3.50-3.70 (1H, brs), 2.87-2.96 (2H, q), 2.36-2.56(1H, m), 2.18-2.35 (1H, m), 1.90-2.05 (1H, m), 1.38 (3H, t), 0.86 (3H, t), 0.75-0.84 (1H, m), 0.40-0.54 (1H, m), 0.15-0.25 (1H, m).

10

Example 38A

Preparation of 1-(1-cyclopropylpropyl)-4-(2,4-dichlorophenyl)-2-ethyl-1H-imidazo[4,5-c]pyridine

15

Part A. A mixture of 4-chloro-3-nitro-2-pyridone (2.0 g, 11.4 mmol), 1-cyclopropylpropyl amine hydrochloride (1.5 g, 11.4 mmol) and N,N-diisopropylethylamine (4.8 ml, 27.4 mmol) in CH₃CN (50 ml) were stirred at 25 °C for 16 h and at reflux for 4h. After cooling it was stripped in vacuo, and the residue was partitioned between EtOAc (100 mL) and H₂O (50 mL). The insolubles were separated, washed with H₂O and EtOAc and vacuum dried 1.51 g. The filtrate layers were separated and the aqueous layer was extracted with EtOAc (2x50 mL). The Combined extracts were washed with brine, dried over MgSO₄, filtered and concd. in vacuo. The residue was washed with EtOAc (2x) and vacuum dried, to give 0.69 g, yellow solid. Combined wt. of 4-(1-cyclopropylpropyl)amino-3-nitro-2-pyridone 2.20 g, 81% yield. ¹H NMR(300 MHz, dmsO d₆): 11.19 (1H, br), 8.94 (1H, d J = 8.8 Hz), 7.33 (1H, t J = 6.9 Hz), 6.03 (1H, d J = 7.7 Hz), 3.18-3.24 (1H, m), 1.60-1.74 (2H, m), 1.03-1.11(1H, m), 0.91 (3H, t), 0.40-0.60 (1H, m), 0.20-0.39 (1H, m).

35

Part B. 4-(1-Cyclopropyl)propylamino-3-nitro-2-pyridone (2.20 g, 9.27 mmol) was stirring in POCl₃ (15 mL) at 25 °C for 16 h. Then it was poured into ice/water (220 mL) and stirred until all the POCl₃ had reacted. The mixture was neutralized

with solid NaHCO_3 , filtered and extracted with EtOAc (3x60 mL). The combined organic extracts were washed with brine, dried over MgSO_4 , filtered and stripped in vacuo. The crude oil was chromatographed on silica gel (100 g.) and eluted with a gradient from 10-20% EtOAc/hexane to afford 1.91 g 2-chloro-4-(1-cyclopropylpropyl)amino-3-nitropyridine, 81% yield. ^1H NMR(300 MHz, CDCl_3): 7.96 (1H, d J = 6.3 Hz), 6.58 (1H, d J = 6.3 Hz), 6.52 (1H, brd J = 5.5 Hz), 2.90-3.00 (1H, m), 1.61-1.82 (2H, m), 1.01 (3H, t J = 7.7 Hz), 0.90-1.02 (1H, m), 0.51-0.70 (2H, m), 0.21-0.34 (2H, m).

Part C. In a dried flask, under N_2 , a mixture of 2-chloro-4-(1-cyclopropyl)propylamino-3-nitropyridine (730 mg, 2.85 mmol), 2,4-dichlorophenylboronic acid (544 mg, 2.85 mmol), dichlorobis(triphenylphosphine) palladium (III) (114 mg, 0.17 mmol) and barium hydroxide octahydrate (899 mg, 2.85 mmol) was heated at reflux in dimethoxyethane (8.6 mL) and H_2O (8.6 mL) for 1.5 h. After cooling it was partitioned between EtOAc (100 mL) and water (20 mL) and filtered through celite. The aqueous layer was extracted with EtOAc (2x50 mL). The combined organics were washed with brine, dried over MgSO_4 , filtered and stripped in vacuo. The residue was chromatographed on silica gel (40 gm), and eluted with 30% EtOAc/hexane to afford a yellow oil, 1.00 g, 90% yield. ^1H NMR(300 MHz, CDCl_3): 8.24 (1H, d J = 6.2 Hz), 7.87 (1H, brd J = 7.3 Hz), 7.43 (1H, s), 7.34 (2H, s), 6.71 (1H, d J = 6.2 Hz), 3.00-3.10 (1H, m), 1.70-1.85 (2H, m), 0.95-1.15 (4H, m), 0.50-0.71 (2H, m), 0.25-0.40 (2H, m).

Part D. The product from Part C (0.94 g, 2.57 mmol), by dissolving in dioxane (26 ml), H_2O (26 ml) and conc. NH_4OH (1.0 ml) while adding $\text{Na}_2\text{S}_2\text{O}_4$ and stirring at room temperature for 2 hrs. Added CH_2Cl_2 and extracted. Extracted the aqueous layer with CH_2Cl_2 (2x). Combined the organics and washed with brine, dried over MgSO_4 , filtered and concd. in vacuo to give a yellow solid, 1.01 g. It was carried over to the next reaction without purification.

Part E. The amine from Part D (1.01 g, 3.00 mmol) was cyclized by refluxing with propionic acid (27 ml, 365.45 mmol) for 8 hrs.. Allowed to cool to RT. then basified with 1M NaOH and 50% NaOH. Extracted with EtOAc (2x60 mL) and CH₂Cl₂ (60 mL). Combined the organics and washed with H₂O, brine, dried over MgSO₄, filtered and concd. in vacuo. The crude oil was chromatographed on silica gel (40 g.) and eluted with 30% EtOAc/hexane to obtain a pale yellow solid (trituated from hexane), 520 mg, 46% yield. ¹H NMR (300 MHz, CDCl₃): 8.43 (1H, d J = 5.8 Hz), 7.63 (1H, d J = 8.1 Hz), 7.55 (1H, d J = 1.8 Hz), 7.46 (1H, d J = 5.8 Hz), 7.36 (1H, dd J = 8.1, 1.8 Hz), 3.40-3.50 (1H, m), 2.80-2.90 (2H, q J = 7.7 Hz), 2.10-2.30 (2H, m), 1.50-1.64 (1H, m), 1.37 (3H, t J = 7.3 Hz), 0.87 (3H, t J = 7.3 Hz), 0.81-0.91 (1H, m), 0.48-0.58 (2H, m), 0.18-0.26 (1H, m). Elemental analysis calcd for C₂₀H₂₁N₃Cl₂: C, 64.18; H, 5.665; N, 11.23; found: C, 64.37; H, 5.66; N, 11.15.

20

Example 831

Preparation of 6-(2-Chloro-4-methoxyphenyl)-9-dicyclopropylmethyl-8-ethylpurine

Part A. A solution of dicyclopropyl ketone (50 g) in absolute methanol (150 mL) in an autoclave vessel was charged with W4 Raney nickel (12 g, washed free of water and in methanol slurry) and then anhydrous ammonia (17 g). The mixture was subjected to 120 atm of hydrogen at 150-160 °C for 5 hours, then cooled and excess gasses purged. The resulting slurry was filtered through celite, and the filtrate was distilled to about one-third the original volume (atmospheric pressure, Vigreux column). The pot solution was cooled to 0 °C, diluted with 3 volumes diethyl ether, and treated with 4 N hydrochloric acid solution in anhydrous dioxane until precipitate formation ceased. The solid product (dicyclopropylmethylamine hydrochloride) was collected by filtration, washed with excess diethyl ether, and dried under vacuum (45.22 g, 306 mmol, 67%). ¹H NMR (300 MHz, methanol-d₄):

d 1.94 (1H, t, $J = 9.3$ Hz), 1.11-0.99 (2H, m), 0.75-0.59 (4H, m), 0.48-0.37 (4H, m). MS (NH_3 -DCI): m/e 114 (5), 113 (100).

Part B. A solution of 5-amino-4,6-dichloropyrimidine (5.00 g, 30.5 mmol) and diisopropylethylamine (12.0 mL, 68.9 mmol) in ethanol (100 mL) was treated with the amine from Part A (3.81 g, 25.8 mmol), and heated to reflux for 72 h. The resulting mixture was cooled and poured into water (300 mL), which was extracted with ethyl acetate (2 x 300 mL). The extracts were washed with brine, combined, dried over sodium sulfate, filtered and evaporated. The residual oil was separated by column chromatography (30:70 ethyl acetate-hexane), and the desired product, 5-amino-4-chloro-6-dicyclopropylmethylaminopyrimidine, was triturated with warm ether-hexane, collected by filtration, and dried under vacuum (3.15 g, 13.2 mmol, 43%). m.p. 137-138 °C. TLC R_f 0.17 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): d 8.01 (1H, s), 4.95 (1H, br d, $J = 7.3$ Hz), 3.45 (1H, q, $J = 7.0$ Hz), 3.37 (2H, br s), 1.06-0.94 (2H, m), 0.59-0.32 (8H, m). MS (NH_3 -CI): m/e 243 (1), 242 (5), 241 (36), 240 (16), 239 (100).

Part C. A solution of the diamine from Part B (1.80 g, 7.54 mmol) and 1 drop concentrated hydrochloric acid in triethyl orthopropionate (12 mL) was heated to 100 °C for 6 hours. The excess orthoester was removed by distillation (partial vacuum, short-path), and the pot residue solidified to give the product, N-(4-chloro-6-dicyclopropylmethylaminopyrimidin-5-yl)-O-ethyl-propionimide. ^1H NMR (300 MHz, CDCl_3): d 8.08 (1H, s), 4.84 (1H, br d, $J = 8.0$ Hz), 4.35 (2H, br), 3.45 (1H, q, $J = 7.7$ Hz), 2.14 (2H, q, $J = 7.3$ Hz), 1.41 (3H, t, $J = 7.1$ Hz), 1.08 (3H, t, $J = 7.7$ Hz), 1.03-0.93 (2H, m), 0.58-0.27 (8H, m). MS (NH_3 -CI): m/e 327 (1), 326 (7), 325 (36), 324 (21), 323 (100).

Part D. A solution of the imide compound prepared in Part C above and p-toluenesulfonic acid monohydrate (50 mg) in diphenyl ether (10 mL) was heated to 170 °C for 2 hours. The resulting mixture was cooled and separated by column

chromatography (silica gel, hexane to remove diphenyl ether, then 30:70 ethyl acetate-hexane) to afford the product, 6-chloro-9-dicyclopropylmethyl-8-ethylpurine, as a solid (1.42 g, 5.13 mmol, 68% for both steps C and D). m.p. 99-100 °C. TLC R_f 0.26 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.63 (1H, s), 2.99 (2H, br), 1.92 (1H, br), 1.50 (3H, t, J = 7.3 Hz), 0.87-0.78 (2H, m), 0.50-0.39 (4H, m), 0.20-0.10 (4H, m). MS ($\text{NH}_3\text{-CI}$): m/e 280 (6), 279 (36), 278 (19), 277 (100).

10 Part E. A solution of 4-amino-3-chlorophenol hydrochloride (18.6 g, 103 mmol) and sodium acetate (18.6 g, 227 mmol) in glacial acetic acid (200 mL) was heated to gentle reflux for 12 hours, then cooled and poured into 4 volumes water. This was neutralized with portionwise addition of sodium
15 bicarbonate, and the resulting mixture was extracted with ethyl acetate (2 x 500 mL). The extracts were washed with brine, combined, dried over magnesium sulfate, filtered and evaporated. The resulting solid was triturated with warm ether; filtration and vacuum drying gave 4-acetamido-3-
20 chlorophenol (16.1 g, 86.7 mmol, 84%). m.p. 128-129 °C. TLC R_f 0.14 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, 4:1 $\text{CDCl}_3\text{:CD}_3\text{OD}$): δ 7.66 (1H, d, J = 8.8 Hz), 6.88 (1H, d, J = 1.7 Hz), 6.74 (1H, dd, J = 8.8, 1.7 Hz), 2.19 (3H, s). MS ($\text{H}_2\text{O-GC/MS}$): m/e 186 (100).

25

Part F. A solution of the phenol of Part E (14.6 g, 78.8 mmol), methyl iodide (10.0 mL, 160 mmol), and sodium carbonate (10.0 g, 94.3 mmol) in acetonitrile (200 mL) was heated to reflux for 48 hours, then cooled and poured into water (800
30 mL). This was extracted with ethyl acetate (2 x 800 mL), and the extracts were washed with brine, combined, dried over magnesium sulfate, filtered and evaporated. The resulting solid was recrystallized from ether-ethyl acetate to afford pure product, 2-chloro-4-methoxyacetanilide (13.2 g, 66.3
35 mmol, 84%), m. p. 118-119 °C (ether-ethyl acetate). TLC R_f 0.30 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.15 (1H, d, J = 9.2 Hz), 7.39 (1H, br s), 6.92 (1H, d, J = 3.0 Hz), 6.82 (1H, dd, J = 9.2, 3.0 Hz), 3.78 (3H, s), 2.22

(3H, s). MS (NH_3 -CI): m/e 219 (19), 217 (60), 202 (40), 201 (14), 200 (100).

Part G. A solution of the amide from Part F (10.1 g, 50.7 mmol) and sodium hydroxide (10 mL, 5 N, 50 mmol) in 95% ethanol (200 mL) was heated to 50 °C for 24 hours. Then, an additional 5 mL sodium hydroxide solution was added, and the mixture was heated to full reflux for an additional 48 hours. The solution was cooled and evaporated, and the residual material was partitioned between ether and water. The aqueous phase was extracted a second time with ether, and the extracts were washed with brine, combined, dried over sodium sulfate, filtered and evaporated. The resulting product, 2-chloro-4-methoxyaniline, was purified by elution through a short column of silica gel with 30:70 ethyl acetate-hexane, and the eluant was evaporated (7.98 g, 100%).

Part H. A solution of the aniline from Part G (7.98 g, 50 mmol) in conc. HCl (25 mL) was cooled to -5 °C, and treated dropwise with a concentrated aqueous solution of sodium nitrite (3.80 g, 55.1 mmol). After 30 minutes, the mixture was charged with 15 mL cyclohexane and 15 mL dichloromethane, then treated dropwise with a concentrated aqueous solution of potassium iodide (16.6 g, 100 mmol). This mixture was allowed to stir for 4 hours, then was extracted with dichloromethane (2 x 100 mL). The extracts were washed in sequence with 1 N aqueous sodium bisulfite (100 mL) and brine (60 mL), then combined, dried over magnesium sulfate, filtered and evaporated to afford sufficiently pure product, 3-chloro-4-iodoanisole (7.00 g, 26.1 mmol, 52%). TLC R_f 0.39 (5:95 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): d 7.69 (1H, d, J = 8.8 Hz), 7.03 (1H, d, J = 3.0 Hz), 6.57 (1H, dd, J = 8.8, 3.0 Hz), 3.78 (3H, s). MS (H_2O -GC/MS): m/e 269 (100).

Part I. A solution of the iodide compound from Part H (7.00 g, 26.1 mmol) in anhydrous tetrahydrofuran (50 mL) was cooled to -90 °C, and treated with a hexane solution of *n*-butyllithium (16.5 mL, 1.6 M, 26.4 mmol). After 15 minutes, the solution

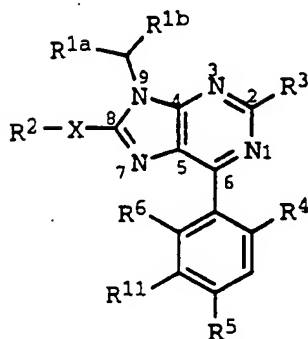
was treated with triisopropylborate (6.10 mL, 26.4 mmol) and was allowed to warm to ambient temperature over 6 hours. The resulting mixture was treated with 6 N aqueous HCl (5 mL) and water (5 mL), which was stirred for 1 hour, then poured into
5 water (100 mL) and extracted with ethyl acetate (2 x 100 mL). The extracts were washed in sequence with 1 N aqueous sodium bisulfite and brine (80 mL each), combined, dried over sodium sulfate, filtered and evaporated. The residual solid was
10 triturated with 1:1 ether-hexane, collected by filtration and dried under vacuum to afford pure product, 2-chloro-4-methoxybenzeneboronic acid (3.05 g, 16.4 mmol, 63%). m.p. 191-195 °C.

Part J. A solution of the chloride from Part D (770 mg, 2.78
15 mmol), the boronic acid from Part I (770 mg, 4.13 mmol), 2 N aqueous sodium carbonate solution (4 mL, 8 mmol) and triphenylphosphine (164 mg, 0.625 mmol) in DME (20 mL) was degassed by repeated cycles of brief vacuum pumping followed by nitrogen purging. To this was added palladium (II) acetate
20 (35 mg, 0.156 mmol), and the mixture was degassed again and then heated to reflux for 14 hours. It was cooled, and poured into water (100 mL). This mixture was extracted with ethyl acetate (2 x 100 mL), and the extracts were washed in sequence with brine (60 mL), combined, dried over sodium sulfate,
25 filtered and evaporated. The residual material was separated by column chromatography (silica gel, 15:85 ethyl acetate-hexane) to afford the title product as a solid. This was recrystallized to purity from hexane (791 mg, 2.07 mmol, 74%). m.p. 139-140 °C (hexane). TLC R_f 0.18 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.93 (1H, s), 7.74 (1H, d, J = 8.4, Hz), 7.10 (1H, d, J = 2.6 Hz), 6.96 (1H, dd, J = 8.4, 2.6 Hz), 4.20 (1H, v br), 3.87 (3H, s), 2.97 (2H, v br), 2.00 (2H, v br), 1.44 (3H, br t, J = 7 Hz), 0.89-0.79 (2H, m), 0.62-0.52 (2H, m), 0.51-0.40 (2H, m), 0.26-0.16 (2H, m). MS
30 ($\text{NH}_3\text{-Cl}$): m/e 387 (1), 386 (9), 385 (41), 384 (30), 383 (100). Analysis calc'd for $\text{C}_{21}\text{H}_{23}\text{ClN}_4\text{O}$: C, 65.87; H, 6.05; N, 14.63; found: C, 65.77; H, 6.03; N, 14.57.

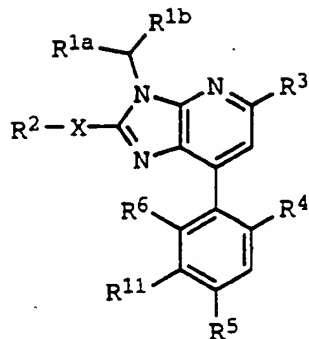
In Table 1, Table 1A and Table 1B, melting point data correspond to compounds of Structure A unless otherwise indicated.

5

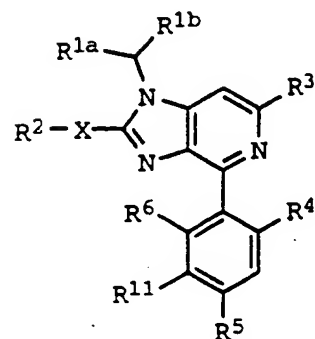
TABLE 1



(A)



(B)



(C)

10

| Ex. No. | R ¹ | X | R ³ | R ⁴ | R ⁵ | R ¹¹ | R ⁶ | R ^{1a} | R ^{1b} | mp, °C. |
|---------|-----------------|-----------------|----------------|-----------------|-----------------|-----------------|-----------------|---------------------------------|--|---------|
| 1 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | 128-129 |
| 2 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | 99-100 |
| 3 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | oil |
| 4 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 5 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₇ | 143-145 |
| 6 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₁₁ | - |
| 7 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | 68-71 |
| 8 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | oil |
| 9 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OH | 196-197 |
| 10 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | oil |
| 11 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^b | oil |
| 12 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 13 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | 120-121 |
| 14 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | (CH ₂) ₂ OH | 209-210 |
| 15 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | H | 140-150 |
| 16 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | c-C ₃ H ₇ | 186-187 |
| 17 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | 121-122 |

| | | | | | | | | | | |
|-----|-----------------|-----------------|---|-----------------|-----------------|---|-----------------|----------------------------------|--|---------|
| 18 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 3-(CH ₃ O)-C ₆ H ₄ | oil |
| 19 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 2-Br-C ₆ H ₄ | 84-85 |
| 20 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 4-CH ₃ -C ₆ H ₄ | 48-50 |
| 21 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 22 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 23 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 3-(C ₆ H ₅)-C ₆ H ₄ | - |
| 24 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | (CH ₃) ₂ OCH ₃ | - |
| 25 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | CH ₃ OCH ₃ | - |
| 26 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₂ H ₅ | 120-123 |
| 27 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₂ H ₅ | oil |
| 28 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | oil |
| 29 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₃ OCH ₃ | - |
| 30 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | OC ₂ H ₅ | 91-93 |
| 31 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | (CH ₃) ₂ CH | 120-121 |
| 32 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | O(CH ₂) ₂ -OCH ₃ | - |
| 33 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 34 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | oil |
| 35 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | oil |
| 36 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₃ OCH ₃ | - |
| 37 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 38 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | c-C ₃ H ₇ | oil |
| (A) | | | | | | | | | | |
| | | | | | | | | | | 118-119 |
| | | | | | | | | | | (B) |
| | | | | | | | | | | 125-126 |
| | | | | | | | | | | (C) |
| 39 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 40 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | oil |
| 41 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 42 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₃ CN | - |
| 43 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ -(Q1) | - |
| 44 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ -(Q2) | - |
| 45 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₃ N(CH ₂) ₂ | - |
| 46 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 47 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | c-C ₃ H ₇ | CH ₃ OCH ₃ | - |
| 48 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | c-C ₃ H ₇ | C ₆ H ₅ | oil |
| 49 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | 156-157 |
| 50 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | C ₆ H ₅ | oil |
| 51 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 3-(CH ₃ O)-C ₆ H ₄ | oil |
| 52 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 2-Br-C ₆ H ₄ | - |

| | | | | | | | | | | |
|----|-----------------|-----------------|---|-----------------|------------------|---|-----------------|----------------------------------|--|---------|
| 53 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 4-CH ₃ -C ₆ H ₄ | 114-115 |
| 54 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 4-C ₆ H ₅ -C ₆ H ₄ | oil |
| 55 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 56 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 3-(C ₆ H ₅)-C ₆ H ₄ | - |
| 57 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | (CH ₂) ₂ OCH ₃ | - |
| 58 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | CH ₂ OCH ₃ | - |
| 59 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | C ₂ H ₅ | - |
| 60 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | C ₃ H ₇ | - |
| 61 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | C ₄ H ₉ | - |
| 62 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 63 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | OC ₂ H ₅ | - |
| 64 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | OC ₂ H ₅ | - |
| 65 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | O(CH ₂) ₂ -OCH ₃ | - |
| 66 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 67 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 68 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | oil |
| 69 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 70 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 71 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 72 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₁₃ | - |
| 73 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 74 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 75 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ CN | - |
| 76 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | - |
| 77 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^c | - |
| 78 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 79 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 80 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | CH ₂ OCH ₃ | - |
| 81 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 82 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | c-C ₃ H ₇ | 167-169 |
| 83 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₆ H ₅ | 134-135 |
| 84 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 3-(CH ₃ O)-C ₆ H ₄ | - |
| 85 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 2-Br-C ₆ H ₄ | - |
| 86 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 4-CH ₃ -C ₆ H ₄ | - |
| 87 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 88 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 89 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 3-(C ₆ H ₅)-C ₆ H ₄ | - |
| 90 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | (CH ₂) ₂ OCH ₃ | - |
| 91 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | CH ₂ OCH ₃ | - |
| 92 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₂ H ₅ | - |

| | | | | | | | | | | |
|-----|-----------------|-----------------|---|-----------------|------------------|---|-----------------|----------------------------------|---|---------|
| 93 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 94 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₄ H ₉ | - |
| 95 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 96 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | OC ₂ H ₅ | - |
| 97 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | OC ₂ H ₅ | - |
| 98 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | O(CH ₂) ₂ -OCH ₃ | - |
| 99 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 100 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | CH ₃ | 138-140 |
| 101 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | 198-199 |
| 102 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | 147-148 |
| 103 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | 140-142 |
| 104 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 105 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 106 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₁₃ | - |
| 107 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 108 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 109 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ CN | - |
| 110 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | - |
| 111 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^c | - |
| 112 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 113 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 114 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | CH ₂ OCH ₃ | - |
| 115 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 116 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 117 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 118 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 3-(CH ₂ O)-C ₆ H ₄ | - |
| 119 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 2-Br-C ₆ H ₄ | - |
| 120 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 4-CH ₃ -C ₆ H ₄ | - |
| 121 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 122 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 3-C ₇ H ₁₅ | oil |
| 123 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | 2-(C ₂ H ₅)-C ₆ H ₁₂ | oil |
| 124 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | (CH ₂) ₃ OCH ₃ | - |
| 125 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | CH ₂ OCH ₃ | - |
| 126 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₂ H ₅ | - |
| 127 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 128 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₄ H ₉ | - |
| 129 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 130 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | OC ₂ H ₅ | - |
| 131 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | OC ₂ H ₅ | - |
| 132 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | O(CH ₂) ₂ -OCH ₃ | - |

| | | | | | | | | | | |
|-----|---|-----------------|---|-----------------|------------------|---|-----------------|----------------------------------|--|---|
| 133 | H | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 134 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 135 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 136 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 137 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 138 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 139 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₁₃ | - |
| 140 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 141 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 142 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ CN | - |
| 143 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ - (Q1) ^b | - |
| 144 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ - (Q2) ^c | - |
| 145 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 146 | H | CH ₂ | H | Cl | Cl | H | H | c-C ₃ H ₇ | C ₄ H ₉ | - |
| 147 | H | CH ₂ | H | Cl | Cl | H | H | c-C ₃ H ₇ | CH ₂ OCH ₃ | - |
| 148 | H | CH ₂ | H | Cl | Cl | H | H | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 149 | H | CH ₂ | H | Cl | Cl | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 150 | H | CH ₂ | H | Cl | Cl | H | H | H | C ₆ H ₅ | - |
| 151 | H | CH ₂ | H | Cl | Cl | H | H | H | 3-(CH ₃ O)-C ₆ H ₄ | - |
| 152 | H | CH ₂ | H | Cl | Cl | H | H | H | 2-Br-C ₆ H ₄ | - |
| 153 | H | CH ₂ | H | Cl | Cl | H | H | H | 4-CH ₃ -C ₆ H ₄ | - |
| 154 | H | CH ₂ | H | Cl | Cl | H | H | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 155 | H | CH ₂ | H | Cl | Cl | H | H | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 156 | H | CH ₂ | H | Cl | Cl | H | H | H | 3-(C ₆ H ₅)-C ₆ H ₄ | - |
| 157 | H | CH ₂ | H | Cl | Cl | H | H | H | (CH ₂) ₂ OCH ₃ | - |
| 158 | H | CH ₂ | H | Cl | Cl | H | H | H | CH ₂ OCH ₃ | - |
| 159 | H | CH ₂ | H | Cl | Cl | H | H | H | C ₂ H ₅ | - |
| 160 | H | CH ₂ | H | Cl | Cl | H | H | H | C ₃ H ₇ | - |
| 161 | H | CH ₂ | H | Cl | Cl | H | H | H | C ₄ H ₉ | - |
| 162 | H | CH ₂ | H | Cl | Cl | H | H | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 163 | H | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | OC ₂ H ₅ | - |
| 164 | H | CH ₂ | H | Cl | Cl | H | H | H | OC ₂ H ₅ | - |
| 165 | H | CH ₂ | H | Cl | Cl | H | H | H | O(CH ₂) ₂ -OCH ₃ | - |
| 166 | H | CH ₂ | H | Cl | Cl | H | H | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 167 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 168 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 169 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 170 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 171 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 172 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₁₃ | - |

| | | | | | | | | | | |
|-----|-----------------|-----------------|---|-----------------|------------------|---|-----------------|----------------------------------|--|--------|
| 173 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 174 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 175 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ CN | - |
| 176 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | - |
| 177 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^c | - |
| 178 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 179 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | C ₆ H ₅ | - |
| 180 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 181 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | C ₆ H ₅ | - |
| 182 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 183 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 184 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 3-(CH ₃ O)-C ₆ H ₄ | - |
| 185 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 2-Br-C ₆ H ₄ | - |
| 186 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 4-CH ₃ -C ₆ H ₄ | - |
| 187 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 188 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 189 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 3-(C ₆ H ₅)-C ₆ H ₄ | - |
| 190 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | (CH ₂) ₂ OCH ₃ | - |
| 191 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | CH ₂ OCH ₃ | - |
| 192 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₂ H ₅ | - |
| 193 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₂ H ₅ | - |
| 194 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 195 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 196 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | OC ₂ H ₅ | - |
| 197 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | OC ₂ H ₅ | - |
| 198 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | H | O(CH ₂) ₂ -OCH ₃ | - |
| 199 | H | CH ₂ | H | CH ₃ | OCH ₃ | H | CH ₃ | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 200 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | C ₂ H ₅ | 98-100 |
| 201 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 202 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | oil |
| 203 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 204 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 205 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 206 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 207 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 208 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 209 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ CN | - |
| 210 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | - |
| 211 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^c | - |
| 212 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |

| | | | | | | | | | | |
|-----|-----------------|---|---|-----------------|-----------------|---|-----------------|----------------------------------|--|---------|
| 213 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | C ₆ H ₅ | - |
| 214 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 215 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | C ₆ H ₅ | - |
| 216 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 217 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 218 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | 3-(CH ₃ O)-C ₆ H ₄ | - |
| 219 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | 2-Br-C ₆ H ₄ | - |
| 220 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | 4-CH ₃ -C ₆ H ₄ | - |
| 221 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 222 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 223 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | 3-(C ₆ H ₅)-C ₆ H ₄ | - |
| 224 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | (CH ₂) ₃ OCH ₃ | - |
| 225 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | CH ₂ OCH ₃ | - |
| 226 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 227 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 228 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 229 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 230 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | OC ₂ H ₅ | - |
| 231 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | OC ₂ H ₅ | - |
| 232 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | O(CH ₂) ₂ -OCH ₃ | - |
| 233 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 234 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 235 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 236 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 237 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 238 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 239 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 240 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 241 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₃ OCH ₃ | - |
| 242 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ CN | - |
| 243 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | - |
| 244 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^c | - |
| 245 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 246 | CH ₃ | O | H | Cl | Cl | H | H | c-C ₃ H ₅ | C ₆ H ₅ | - |
| 247 | CH ₃ | O | H | Cl | Cl | H | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 248 | CH ₃ | O | H | Cl | Cl | H | H | c-C ₃ H ₅ | C ₆ H ₅ | - |
| 249 | CH ₃ | O | H | Cl | Cl | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 132-134 |
| 250 | CH ₃ | O | H | Cl | Cl | H | H | H | C ₆ H ₅ | - |
| 251 | CH ₃ | O | H | Cl | Cl | H | H | H | 3-(CH ₃ O)-C ₆ H ₄ | - |
| 252 | CH ₃ | O | H | Cl | Cl | H | H | H | 2-Br-C ₆ H ₄ | - |

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|-----|-----------------|---|---|-----------------|------------------|---|-----------------|----------------------------------|---|---|
| 253 | CH ₃ | O | H | Cl | Cl | H | H | H | 4-CH ₃ -C ₆ H ₄ | - |
| 254 | CH ₃ | O | H | Cl | Cl | H | H | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 255 | CH ₃ | O | H | Cl | Cl | H | H | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 256 | CH ₃ | O | H | Cl | Cl | H | H | H | 3-(C ₆ H ₅)-C ₆ H ₁₀ | - |
| 257 | CH ₃ | O | H | Cl | Cl | H | H | H | (CH ₂) ₂ OCH ₃ | - |
| 258 | CH ₃ | O | H | Cl | Cl | H | H | H | CH ₂ OCH ₃ | - |
| 259 | CH ₃ | O | H | Cl | Cl | H | H | H | C ₂ H ₅ | - |
| 260 | CH ₃ | O | H | Cl | Cl | H | H | H | C ₃ H ₇ | - |
| 261 | CH ₃ | O | H | Cl | Cl | H | H | H | C ₄ H ₉ | - |
| 262 | CH ₃ | O | H | Cl | Cl | H | H | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 263 | CH ₃ | O | H | Cl | Cl | H | H | C ₂ H ₅ | OC ₂ H ₅ | - |
| 264 | CH ₃ | O | H | Cl | Cl | H | H | H | OC ₂ H ₅ | - |
| 265 | CH ₃ | O | H | Cl | Cl | H | H | H | O(CH ₂) ₂ -OCH ₃ | - |
| 266 | CH ₃ | O | H | Cl | Cl | H | H | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 267 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 268 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 269 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 270 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 271 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 272 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₁₃ | - |
| 273 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 274 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 275 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ CN | - |
| 276 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | - |
| 277 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^c | - |
| 278 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 279 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 280 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | CH ₂ OCH ₃ | - |
| 281 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 282 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 283 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 284 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 3-(CH ₃ O)-C ₆ H ₄ | - |
| 285 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 2-Br-C ₆ H ₄ | - |
| 286 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 4-CH ₃ -C ₆ H ₄ | - |
| 287 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 288 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 289 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 3-(C ₆ H ₅)-C ₆ H ₁₀ | - |
| 290 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | (CH ₂) ₂ OCH ₃ | - |
| 291 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | CH ₂ OCH ₃ | - |
| 292 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₂ H ₅ | - |

| | | | | | | | | | | |
|-----|-----------------|-----------------|-----------------|-----------------|------------------|---|-----------------|----------------------------------|--|---------|
| 293 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 294 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₄ H ₉ | - |
| 295 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 296 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | OC ₂ H ₅ | - |
| 297 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | OC ₂ H ₅ | - |
| 298 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | H | O(CH ₂) ₂ -OCH ₃ | - |
| 299 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | CH ₃ | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 300 | CH ₃ | CH ₂ | CH ₃ | H | Cl | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | 106-109 |
| 301 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 302 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 303 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 304 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 305 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 306 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₁₃ | - |
| 307 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 308 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 309 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ CN | - |
| 310 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | - |
| 311 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^c | - |
| 312 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 313 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 314 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | CH ₂ OCH ₃ | - |
| 315 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 316 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 317 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 318 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | 3-(CH ₃ O)-C ₆ H ₄ | - |
| 319 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | 2-Br-C ₆ H ₄ | - |
| 320 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | 4-CH ₃ -C ₆ H ₄ | - |
| 321 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 322 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 323 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | 3-(C ₆ H ₅)-C ₆ H ₄ | - |
| 324 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | (CH ₂) ₂ OCH ₃ | - |
| 325 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | CH ₂ OCH ₃ | - |
| 326 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₂ H ₅ | - |
| 327 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 328 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 329 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 330 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | OC ₂ H ₅ | - |
| 331 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | OC ₂ H ₅ | - |
| 332 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | H | O(CH ₂) ₂ -OCH ₃ | - |

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|-----|-----------------|---|---|-----------------|------------------|---|-----------------|----------------------------------|--|---|
| 333 | CH ₃ | S | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 334 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 335 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 336 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 337 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 338 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | c-C ₂ H ₅ | - |
| 339 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 340 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 341 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₃) ₂ OCH ₃ | - |
| 342 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ CN | - |
| 343 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | - |
| 344 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^c | - |
| 345 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 346 | CH ₃ | S | H | Cl | Cl | H | H | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 347 | CH ₃ | S | H | Cl | Cl | H | H | c-C ₃ H ₇ | CH ₂ OCH ₃ | - |
| 348 | CH ₃ | S | H | Cl | Cl | H | H | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 349 | CH ₃ | S | H | Cl | Cl | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 350 | CH ₃ | S | H | Cl | Cl | H | H | H | C ₆ H ₅ | - |
| 351 | CH ₃ | S | H | Cl | Cl | H | H | H | 3-(CH ₃ O)-C ₆ H ₄ | - |
| 352 | CH ₃ | S | H | Cl | Cl | H | H | H | 2-Br-C ₆ H ₄ | - |
| 353 | CH ₃ | S | H | Cl | Cl | H | H | H | 4-CH ₃ -C ₆ H ₄ | - |
| 354 | CH ₃ | S | H | Cl | Cl | H | H | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 355 | CH ₃ | S | H | Cl | Cl | H | H | H | 2-(C ₆ H ₅)-C ₆ H ₄ | - |
| 356 | CH ₃ | S | H | Cl | Cl | H | H | H | 3-(C ₆ H ₅)-C ₆ H ₄ | - |
| 357 | CH ₃ | S | H | Cl | Cl | H | H | H | (CH ₂) ₂ OCH ₃ | - |
| 358 | CH ₃ | S | H | Cl | Cl | H | H | H | CH ₂ OCH ₃ | - |
| 359 | CH ₃ | S | H | Cl | Cl | H | H | H | C ₂ H ₅ | - |
| 360 | CH ₃ | S | H | Cl | Cl | H | H | H | C ₃ H ₇ | - |
| 361 | CH ₃ | S | H | Cl | Cl | H | H | H | C ₄ H ₉ | - |
| 362 | CH ₃ | S | H | Cl | Cl | H | H | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 363 | CH ₃ | S | H | Cl | Cl | H | H | C ₂ H ₅ | OC ₂ H ₅ | - |
| 364 | CH ₃ | S | H | Cl | Cl | H | H | H | OC ₂ H ₅ | - |
| 365 | CH ₃ | S | H | Cl | Cl | H | H | H | O(CH ₂) ₃ -OCH ₃ | - |
| 366 | CH ₃ | S | H | Cl | Cl | H | H | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 367 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 368 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 369 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 370 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 371 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 372 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |

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|-----|-----------------|-----------------|-----------------|-----------------|------------------|---|-----------------|----------------------------------|--|---------|
| 373 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 374 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 375 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ CN | - |
| 376 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q1) ^b | - |
| 377 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ -(Q2) ^c | - |
| 378 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ N(CH ₃) ₂ | - |
| 379 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 380 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | CH ₂ OCH ₃ | - |
| 381 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 382 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 383 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 384 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 3-(CH ₃ O)-C ₆ H ₄ | - |
| 385 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 2-Br-C ₆ H ₄ | - |
| 386 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 4-CH ₃ -C ₆ H ₄ | - |
| 387 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 4-C ₆ H ₅ -C ₆ H ₄ | - |
| 388 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 2-(C ₆ H ₅)-C ₆ H ₅ | - |
| 389 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | 3-(C ₆ H ₅)-C ₆ H ₅ | - |
| 390 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | (CH ₂) ₂ OCH ₃ | - |
| 391 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | CH ₂ OCH ₃ | - |
| 392 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₂ H ₅ | - |
| 393 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 394 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | C ₄ H ₉ | - |
| 395 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 396 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | OC ₂ H ₅ | - |
| 397 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | OC ₂ H ₅ | - |
| 398 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | H | O(CH ₂) ₂ -OCH ₃ | - |
| 399 | CH ₃ | S | H | CH ₃ | OCH ₃ | H | CH ₃ | CH ₂ OCH ₃ | C ₆ H ₅ | - |
| 400 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | C ₃ H ₇ | c-C ₃ H ₇ | 153-156 |
| 401 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 402 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | 107-108 |
| 403 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | c-C ₃ H ₇ | 187-188 |
| 404 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | oil |
| 405 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | 98-99 |
| 406 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | 149-150 |
| 407 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 408 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | H | (CH ₂) ₂ OCH ₃ | - |
| 409 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 410 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 411 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 412 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | c-C ₃ H ₇ | C ₆ H ₅ | - |

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|-----|-----------------|-----------------|---|-----------------|------------------|---|------------------|----------------------------------|---|--------------|
| 413 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 139-140 |
| 414 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | CH ₃ | C ₃ H ₇ | oil (A,C) |
| 415 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₂ H ₅ | C ₄ H ₉ | oil |
| 416 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | H | C ₆ H ₅ | - |
| 417 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 418 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | H | (CH ₂) ₂ OCH ₃ | - |
| 419 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 420 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 421 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 422 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 423 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 177-178 |
| 424 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | CH ₃ | C ₃ H ₇ | oil |
| 425 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 426 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | H | C ₆ H ₅ | - |
| 427 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 428 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | H | (CH ₂) ₂ OCH ₃ | - |
| 429 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 430 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 431 | CH ₃ | CH ₂ | H | Cl | Cl | H | OCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | 141-144 |
| 432 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | OCH ₃ | C ₂ H ₅ | C ₃ H ₇ | 108-110 |
| 433 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | 194-195 |
| 434 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₅ CH ₂ | oil |
| 435 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OH | 155-157 |
| 436 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₅ CH ₂ | oil |
| 437 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | CH ₃ | C ₃ H ₇ | oil |
| 438 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | H | 4-(CH ₂ O)-C ₆ H ₅ | oil |
| 439 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₅ | oil |
| 440 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | CH ₃ | C ₃ H ₁₁ | oil |
| 441 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 442 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 443 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 444 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | H | C ₃ H ₇ | - |
| 445 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 446 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | H | C ₆ H ₅ | - |
| 447 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 448 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | H | (CH ₂) ₂ OCH ₃ | - |
| 449 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 450 | CH ₃ | CH ₂ | H | Cl | NMe ₂ | H | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 451 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | C ₂ H ₅ | C ₂ H ₅ | - |

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|-----|-------------------------------|-------------------|------------------|-----------------|------------------|---|-----------------|----------------------------------|--|-------|
| 452 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 453 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 454 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | H | C ₃ H ₇ | - |
| 455 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 456 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | H | C ₄ H ₉ | - |
| 457 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 458 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | H | (CH ₂) ₂ OCH ₃ | - |
| 459 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 460 | CH ₃ | CH ₂ | H | CH ₃ | NMe ₂ | H | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 461 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 462 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 463 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 464 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 465 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 466 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | H | C ₄ H ₉ | - |
| 467 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 468 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | H | (CH ₂) ₂ OCH ₃ | - |
| 469 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 470 | CH ₃ | CH ₂ | NMe ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 471 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 472 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 473 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 474 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 475 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | 92-95 |
| 476 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₄ H ₉ | - |
| 477 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 478 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | (CH ₂) ₂ OCH ₃ | - |
| 479 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 480 | C ₂ H ₅ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 481 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | - |
| 482 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 483 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 484 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₃ H ₇ | - |
| 485 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 486 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | H | C ₄ H ₉ | - |
| 487 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 488 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | H | (CH ₂) ₂ OCH ₃ | - |
| 489 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 490 | CH ₃ | CHCH ₃ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 491 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | 96-97 |

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|-----|-----------------|-----------------|---|------------------|------------------|---|-----------------|----------------------------------|--|--|
| 492 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | c-C ₃ H ₇ | C ₄ H ₉ | - |
| 493 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | 149-150 |
| 494 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | H | C ₃ H ₇ | 99-100 |
| 495 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 496 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | H | C ₄ H ₉ | - |
| 497 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 498 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | H | (CH ₂) ₂ OCH ₃ | - |
| 499 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | CH ₂ OCH ₃ | CH ₂ OCH ₃ | - |
| 500 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 501 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 502 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | C ₃ H ₇ | oil |
| 503 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | C ₃ H ₁₁ | oil |
| 504 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | 2-C ₂ H ₅ | 109-110 |
| 505 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OC ₂ H ₅ | - |
| 506 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | C ₃ H ₇ | oil (A,B,C) |
| 507 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | C ₄ H ₉ | oil |
| 508 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | C ₃ H ₁₁ | - |
| 509 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | 2-C ₂ H ₅ | - |
| 510 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ OC ₂ H ₅ | - |
| 511 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₇ | oil (A) 78-80 (B) 116-117 (C) |
| 512 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | 145-146 |
| 513 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | oil |
| 514 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | oil |
| 515 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ OC ₂ H ₅ | - |
| 516 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 517 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | c-C ₃ H ₇ | c-C ₃ H ₇ | 183-184 |
| 518 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | C ₄ H ₉ | 109-110 |
| 519 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 520 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | CH ₂ OC ₂ H ₅ | - |
| 521 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | C ₃ H ₇ | 115-120 |
| 522 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 523 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₃ H ₇ | C ₃ H ₇ | 99-101 |
| 524 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | oil |
| 525 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | C ₃ H ₇ | 109-111 |

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|-----|-----------------|-----------------|---|------------------|------------------|-----------------|-----------------|-------------------------------|---|---------|
| 526 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₃ H ₇ | C ₃ H ₇ | oil |
| 527 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 528 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | oil |
| 529 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | C ₃ H ₇ | C ₃ H ₇ | - |
| 530 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | C ₃ H ₇ | C ₃ H ₇ | 129-131 |
| 531 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | (CH ₃) ₂ CHCH ₂ | 77-85 |
| 532 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | (CH ₃) ₂ CHCH ₂ | - |
| 533 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | (CH ₃) ₂ CHCH ₂ | - |
| 534 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | CH ₃ | (CH ₃) ₂ CHCH ₂ | - |
| 535 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | CH ₃ | (CH ₃) ₂ CHCH ₂ | - |
| 536 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | CH ₃ | (CH ₃) ₂ CHCH ₂ | - |
| 537 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | (CH ₃) ₂ CHCH ₂ | - |
| 538 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | (CH ₃) ₂ CH | oil |
| 539 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | CH ₃ | (CH ₃) ₂ CHCH ₂ | - |
| 540 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | CH ₃ | (CH ₃) ₂ CHCH ₂ | - |
| 541 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | c-C ₃ H ₇ | 118-127 |
| 542 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | c-C ₃ H ₇ | - |
| 543 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | c-C ₃ H ₇ | oil |
| 544 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | CH ₃ | c-C ₃ H ₇ | oil |
| 545 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | CH ₃ | c-C ₃ H ₇ | - |
| 546 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | CH ₃ | c-C ₃ H ₇ | - |
| 547 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | - |
| 548 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | CH ₃ | c-C ₃ H ₇ | oil |
| 549 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | CH ₃ | c-C ₃ H ₇ | - |
| 550 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | CH ₃ | c-C ₃ H ₇ | - |
| 551 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | CH ₃ | oil |
| 552 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | CH ₃ | - |
| 553 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | CH ₃ | - |
| 554 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | CH ₃ | CH ₃ | - |
| 555 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | CH ₃ | CH ₃ | - |
| 556 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | CH ₃ | CH ₃ | - |
| 557 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | - |
| 558 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | CH ₃ | C ₄ H ₉ | oil |
| 559 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | CH ₃ | CH ₃ | - |
| 560 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | CH ₃ | CH ₃ | - |
| 561 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₁₁ | 102-103 |
| 562 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₁₁ | - |
| 563 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₃ H ₁₁ | - |
| 564 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | oil |
| 565 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₁₁ | - |

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|-----|-----------------|-----------------|---|------------------|------------------|-----------------|-----------------|-------------------------------|--|-----|
| 566 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₂ H ₅ | C ₃ H ₁₁ | - |
| 567 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | C ₂ H ₅ | C ₃ H ₁₁ | - |
| 568 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | C ₃ H ₁₁ | - |
| 569 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | C ₂ H ₅ | C ₃ H ₁₁ | - |
| 570 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | C ₃ H ₁₁ | - |
| 571 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | oil |
| 572 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | - |
| 573 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | - |
| 574 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | - |
| 575 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | - |
| 576 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | - |
| 577 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | - |
| 578 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | - |
| 579 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | - |
| 580 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | C ₂ H ₅ O(CH ₂) ₂ | - |
| 581 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | oil |
| 582 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | - |
| 583 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | - |
| 584 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | - |
| 585 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | - |
| 586 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | - |
| 587 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | - |
| 588 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | - |
| 589 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | - |
| 590 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | C ₂ H ₅ OCH ₂ | - |
| 591 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | H | c-C ₃ H ₇ CH(OMe) (CH ₂) ₂ | oil |
| 592 | CH ₃ | O | H | CH ₃ | CH ₃ | H | CH ₃ | H | c-C ₃ H ₇ CH(OMe) (CH ₂) ₂ | - |
| 593 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | c-C ₃ H ₇ CH(OMe) (CH ₂) ₂ | - |
| 594 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | H | c-C ₃ H ₇ CH(OMe) (CH ₂) ₂ | - |
| 595 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | H | c-C ₃ H ₇ CH(OMe) (CH ₂) ₂ | - |
| 596 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | H | c-C ₃ H ₇ CH(OMe) (CH ₂) ₂ | - |
| 597 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | H | c-C ₃ H ₇ CH(OMe) (CH ₂) ₂ | - |
| 598 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | H | c-C ₃ H ₇ CH(OMe) | - |

| | | | | | | | | | | |
|-----|-----------------|-----------------|-----------------|------------------|------------------|---|-----------------|---------------------------------|--|---------|
| | | | | | | | | | (CH ₂) ₂ | |
| 599 | CH ₃ | CH ₃ | H | Cl | CF ₃ | H | Cl | H | c-C ₃ H ₅ CH(OMe) | - |
| | | | | | | | | | (CH ₂) ₂ | |
| 600 | CH ₃ | CH ₃ | H | OCH ₃ | Cl | H | Cl | H | c-C ₃ H ₅ CH(OMe) | - |
| | | | | | | | | | (CH ₂) ₂ | |
| 601 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 602 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 603 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 155-156 |
| 604 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | H | C ₄ H ₉ | - |
| 605 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 606 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | H | C ₄ H ₉ | - |
| 607 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 608 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | CH ₃ | C ₄ H ₉ | - |
| 609 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 610 | CH ₃ | CH ₃ | CH ₃ | Cl | Cl | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 611 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 612 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 613 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 614 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | H | C ₄ H ₉ | - |
| 615 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 616 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | H | C ₄ H ₉ | - |
| 617 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 618 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | CH ₃ | C ₄ H ₉ | - |
| 619 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 620 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 621 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 622 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 623 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 624 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | H | C ₄ H ₉ | - |
| 625 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 626 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | H | C ₄ H ₉ | - |
| 627 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 628 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | CH ₃ | C ₄ H ₉ | - |
| 629 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 630 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 631 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | Cl | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 632 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | Cl | H | H | c-C ₃ H ₅ | C ₄ H ₉ | - |
| 633 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | Cl | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 634 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | Cl | H | H | H | C ₄ H ₉ | - |
| 635 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | Cl | H | H | C ₂ H ₅ | C ₄ H ₉ | - |

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|-----|-----------------|-----------------|-----------------|------------------|-----------------|---|----|---------------------------------|--|---|
| 636 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | Cl | H | H | H | C ₆ H ₅ | - |
| 637 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | Cl | H | H | C ₂ H ₅ | (CH ₃) ₂ OCH ₃ | - |
| 638 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | Cl | H | H | CH ₃ | C ₄ H ₉ | - |
| 639 | CH ₃ | CH ₃ | CH ₃ | CH ₃ | Cl | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 640 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | Cl | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 641 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 642 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | H | c-C ₃ H ₇ | C ₄ H ₉ | - |
| 643 | CH ₃ | CH ₃ | CH ₃ | Cl | CF ₃ | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 644 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | H | H | C ₄ H ₉ | - |
| 645 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 646 | CH ₃ | CH ₃ | CH ₃ | Cl | CF ₃ | H | H | H | C ₆ H ₅ | - |
| 647 | CH ₃ | CH ₃ | CH ₃ | Cl | CF ₃ | H | H | C ₂ H ₅ | (CH ₃) ₂ OCH ₃ | - |
| 648 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | H | CH ₃ | C ₄ H ₉ | - |
| 649 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 650 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 651 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | Cl | C ₂ H ₅ | C ₃ H ₇ | - |
| 652 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | Cl | c-C ₃ H ₇ | C ₄ H ₉ | - |
| 653 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | Cl | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 654 | CH ₃ | CH ₃ | CH ₃ | Cl | CF ₃ | H | Cl | H | C ₄ H ₉ | - |
| 655 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | Cl | C ₂ H ₅ | C ₄ H ₉ | - |
| 656 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | Cl | H | C ₆ H ₅ | - |
| 657 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | Cl | C ₂ H ₅ | (CH ₃) ₂ OCH ₃ | - |
| 658 | CH ₃ | CH ₃ | CH ₃ | Cl | CF ₃ | H | Cl | CH ₃ | C ₄ H ₉ | - |
| 659 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | Cl | C ₃ H ₇ | C ₃ H ₇ | - |
| 660 | CH ₃ | CH ₂ | CH ₃ | Cl | CF ₃ | H | Cl | C ₂ H ₅ | C ₃ H ₇ | - |
| 661 | CH ₃ | CH ₂ | CH ₃ | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | C ₃ H ₇ | - |
| 662 | CH ₃ | CH ₂ | CH ₃ | OCH ₃ | Cl | H | Cl | c-C ₃ H ₇ | C ₄ H ₉ | - |
| 663 | CH ₃ | CH ₂ | CH ₃ | OCH ₃ | Cl | H | Cl | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 664 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | Cl | H | Cl | H | C ₄ H ₉ | - |
| 665 | CH ₃ | CH ₂ | CH ₃ | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | C ₄ H ₉ | - |
| 666 | CH ₃ | CH ₂ | CH ₃ | OCH ₃ | Cl | H | Cl | H | C ₆ H ₅ | - |
| 667 | CH ₃ | CH ₂ | CH ₃ | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | (CH ₃) ₂ OCH ₃ | - |
| 668 | CH ₃ | CH ₃ | CH ₃ | OCH ₃ | Cl | H | Cl | CH ₃ | C ₄ H ₉ | - |
| 669 | CH ₃ | CH ₂ | CH ₃ | OCH ₃ | Cl | H | Cl | C ₃ H ₇ | C ₃ H ₇ | - |
| 670 | CH ₃ | CH ₂ | CH ₃ | OCH ₃ | Cl | H | Cl | C ₂ H ₅ | C ₃ H ₇ | - |
| 671 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 672 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | c-C ₃ H ₇ | C ₄ H ₉ | - |
| 673 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 674 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | H | C ₄ H ₉ | - |
| 675 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |

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|-----|-----------------|-----------------|-----------------|------------------|------------------|-----------------|-----------------|---------------------------------|--|---------|
| 676 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | H | C ₆ H ₅ | - |
| 677 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | C ₂ H ₅ | (CH ₂) ₂ OCH ₃ | - |
| 678 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | CH ₃ | C ₆ H ₅ | - |
| 679 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 680 | CH ₃ | CH ₂ | CH ₃ | CH ₃ | CH ₃ | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 681 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 682 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | C ₆ H ₅ | 107-109 |
| 683 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | C ₂ H ₅ | C ₆ H ₅ | - |
| 684 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 685 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | 101-103 |
| 686 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | c-C ₃ H ₇ | 187-188 |
| 687 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 688 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | c-C ₃ H ₇ | c-C ₃ H ₇ | 119-121 |
| 689 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | H | C ₆ H ₅ | 108-109 |
| 690 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | oil |
| 691 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | H | C ₆ H ₅ | - |
| 692 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | H | C ₆ H ₅ | oil |
| 693 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₇ | C ₆ H ₅ | oil |
| 694 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 695 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 696 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 697 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | CH ₃ | C ₆ H ₅ | oil |
| 698 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | CH ₃ | CH ₃ | C ₆ H ₅ | - |
| 699 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | Cl | CH ₃ | C ₆ H ₅ | - |
| 700 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | C ₆ H ₅ | - |
| 701 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 702 | CH ₃ | O | H | OCH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | C ₆ H ₅ | - |
| 703 | CH ₃ | O | H | Cl | CF ₃ | H | Cl | C ₂ H ₅ | C ₆ H ₅ | - |
| 704 | CH ₃ | O | H | CH ₃ | CH ₃ | CH ₃ | H | C ₂ H ₅ | C ₆ H ₅ | - |
| 705 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 706 | CH ₃ | O | H | OCH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 707 | CH ₃ | O | H | Cl | CF ₃ | H | Cl | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 708 | CH ₃ | O | H | CH ₃ | CH ₃ | CH ₃ | H | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 709 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | H | H | C ₆ H ₅ | - |
| 710 | CH ₃ | O | H | OCH ₃ | CH ₃ | H | CH ₃ | H | C ₆ H ₅ | - |
| 711 | CH ₃ | O | H | Cl | CF ₃ | H | Cl | H | C ₆ H ₅ | - |
| 712 | CH ₃ | O | H | CH ₃ | CH ₃ | CH ₃ | H | H | C ₆ H ₅ | - |
| 713 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 714 | CH ₃ | O | H | OCH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₇ | C ₆ H ₅ | - |
| 715 | CH ₃ | O | H | Cl | CF ₃ | H | Cl | c-C ₃ H ₇ | C ₆ H ₅ | - |

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|-------|-----------------|-----------------|---|------------------|------------------|------------------|-----------------|---------------------------------|-----------------------------------|---------|
| 716 | CH ₃ | O | H | CH ₃ | CH ₃ | CH ₃ | H | c-C ₃ H ₇ | C ₄ H ₉ | - |
| 717 | CH ₃ | O | H | CH ₃ | OCH ₃ | H | H | CH ₃ | C ₄ H ₉ | - |
| 718 | CH ₃ | O | H | OCH ₃ | CH ₃ | H | CH ₃ | CH ₃ | C ₄ H ₉ | - |
| 719 | CH ₃ | O | H | Cl | CF ₃ | H | Cl | CH ₃ | C ₄ H ₉ | - |
| 720 | CH ₃ | O | H | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 721 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH(CH ₃) ₂ | 146-147 |
| 722 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 723 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 724 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₂ H ₅ | CH(CH ₃) ₂ | oil |
| 725 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | CH(CH ₃) ₂ | oil |
| 726 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 727 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | C ₂ H ₅ | CH(CH ₃) ₂ | oil |
| 728 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 729 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 730 | CH ₃ | CH ₂ | H | Cl | CN | H | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 731 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 732 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 733 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 734 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 735 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 736 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 737 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 738 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 739 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 740 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 741 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 742 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 743 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 744 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 745 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 746 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | C ₂ H ₅ | CH(CH ₃) ₂ | - |
| 747 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | c-C ₃ H ₇ | 140-143 |
| 748 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₃ H ₇ | c-C ₃ H ₇ | 107-108 |
| (A) | | | | | | | | | | |
| 79-82 | | | | | | | | | | |
| (C) | | | | | | | | | | |
| 749 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₃ H ₇ | c-C ₃ H ₇ | 106-108 |
| 750 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₃ H ₇ | c-C ₃ H ₇ | oil |
| 751 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | c-C ₃ H ₇ | oil |
| 752 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₃ H ₇ | c-C ₃ H ₇ | 108-109 |

| | | | | | | | | | | |
|-----|-----------------|-----------------|---|-----------------|------------------|------------------|-----------------|-------------------------------|---------------------------------|----------------------------|
| 753 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | C ₃ H ₇ | c-C ₃ H ₅ | oil (A) 95-97 (C) |
| 754 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₃ H ₇ | c-C ₃ H ₅ | 87-88 |
| 755 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 756 | CH ₃ | CH ₂ | H | Cl | CN | H | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 757 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 758 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 759 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 760 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 761 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 762 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 763 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 764 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 765 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 766 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 767 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | c-C ₃ H ₅ | oil |
| 768 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 769 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 770 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 771 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 772 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 773 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | CH ₂ Cl | 109-110 |
| 774 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 775 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 776 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₃ H ₅ | C ₃ H ₇ | oil |
| 777 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₃ H ₅ | C ₃ H ₇ | oil |
| 778 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₃ H ₅ | C ₃ H ₇ | oil |
| 779 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | C ₃ H ₅ | C ₃ H ₇ | oil |
| 780 | CH ₃ | CH ₂ | H | CH ₃ | Cl | H | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 781 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 782 | CH ₃ | CH ₂ | H | Cl | CN | H | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 783 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 784 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 785 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 786 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 787 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 788 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | C ₃ H ₅ | C ₃ H ₇ | - |
| 789 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | C ₃ H ₅ | C ₃ H ₇ | - |

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|---------|-----------------|-----------------|---|-----------------|------------------|------------------|---|---------------------------------|---|---------|
| 790 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 791 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 792 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 793 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | C ₃ H ₇ | oil |
| 794 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 795 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 796 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 797 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 798 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 799 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | C ₂ H ₅ | C ₃ H ₇ | oil |
| 800 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | H | 4-CH ₃ O-C ₆ H ₄ | 138-139 |
| 801 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 138-139 |
| 802 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | C ₂ H ₅ | c-C ₃ H ₅ | oil |
| (A) | | | | | | | | | | |
| 122-125 | | | | | | | | | | |
| (C) | | | | | | | | | | |
| 803 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | CH ₃ | c-C ₃ H ₅ | oil |
| 804 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | CH ₃ | C ₃ H ₇ | oil |
| 805 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | CH ₃ | C ₄ H ₉ | oil |
| 806 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | CH ₃ | C ₃ H ₁₁ | - |
| 807 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | C ₂ H ₅ | C ₄ H ₉ | oil |
| 808 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | C ₃ H ₇ | C ₃ H ₇ | oil |
| 809 | CH ₃ | CH ₂ | H | CF ₃ | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | oil |
| 810 | CH ₃ | CH ₂ | H | Cl | CN | H | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 811 | CH ₃ | CH ₂ | H | Cl | CN | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 180-182 |
| 812 | CH ₃ | CH ₂ | H | Cl | CN | H | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 813 | CH ₃ | CH ₂ | H | Cl | CN | H | H | CH ₃ | c-C ₃ H ₅ | - |
| 814 | CH ₃ | CH ₂ | H | Cl | CN | H | H | CH ₃ | C ₃ H ₇ | - |
| 815 | CH ₃ | CH ₂ | H | Cl | CN | H | H | CH ₃ | C ₄ H ₉ | - |
| 816 | CH ₃ | CH ₂ | H | Cl | CN | H | H | CH ₃ | C ₃ H ₁₁ | - |
| 817 | CH ₃ | CH ₂ | H | Cl | CN | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 818 | CH ₃ | CH ₂ | H | Cl | CN | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 819 | CH ₃ | CH ₂ | H | Cl | CN | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 820 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 821 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 149-150 |
| 822 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 823 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | CH ₃ | c-C ₃ H ₅ | - |
| 824 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | CH ₃ | C ₃ H ₇ | oil |
| 825 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | CH ₃ | C ₄ H ₉ | - |
| 826 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | CH ₃ | C ₃ H ₁₁ | - |

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|-----|-----------------|-----------------|---|-----------------|------------------|----|---|---------------------------------|---|---------|
| 827 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 828 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 829 | CH ₃ | CH ₂ | H | CF ₃ | CF ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 830 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | 58-60 |
| 831 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 139-140 |
| 832 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₅ | oil |
| 833 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | H | c-C ₃ H ₅ | oil |
| 834 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | CH ₃ | C ₃ H ₇ | oil |
| 835 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | CH ₃ | C ₄ H ₉ | oil |
| 836 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | CH ₃ | C ₃ H ₁₁ | oil |
| 837 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | oil |
| 838 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | oil |
| 839 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | oil |
| 840 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 841 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 148-149 |
| 842 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 843 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | CH ₃ | c-C ₃ H ₅ | - |
| 844 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | CH ₃ | C ₃ H ₇ | - |
| 845 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | CH ₃ | C ₄ H ₉ | - |
| 846 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | CH ₃ | C ₃ H ₁₁ | - |
| 847 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 848 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 849 | CH ₃ | CH ₂ | H | Cl | Cl | F | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 850 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 851 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 852 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 853 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | CH ₃ | c-C ₃ H ₅ | - |
| 854 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | CH ₃ | C ₃ H ₇ | - |
| 855 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | CH ₃ | C ₄ H ₉ | - |
| 856 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | CH ₃ | C ₃ H ₁₁ | - |
| 857 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 858 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 859 | CH ₃ | CH ₂ | H | Cl | Cl | Cl | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 860 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 861 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 128-129 |
| 862 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 863 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | CH ₃ | c-C ₃ H ₅ | - |
| 864 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | CH ₃ | C ₃ H ₇ | - |
| 865 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | CH ₃ | C ₄ H ₉ | - |
| 866 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | CH ₃ | C ₃ H ₁₁ | - |

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|-----|-----------------|-----------------|---|-----------------|------------------|----|---|---------------------------------|---|---------|
| 867 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 868 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 869 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 870 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 4-CH ₃ O-C ₆ H ₄ | oil |
| 871 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | c-C ₃ H ₇ | c-C ₃ H ₇ | 179-181 |
| 872 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 873 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | CH ₃ | c-C ₃ H ₇ | - |
| 874 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | CH ₃ | C ₂ H ₅ | - |
| 875 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | CH ₃ | C ₂ H ₅ | - |
| 876 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | CH ₃ | C ₂ H ₁₁ | - |
| 877 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 878 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 879 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 880 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 881 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | c-C ₃ H ₇ | c-C ₃ H ₇ | 130-131 |
| 882 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 883 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | CH ₃ | c-C ₃ H ₇ | - |
| 884 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | CH ₃ | C ₂ H ₅ | - |
| 885 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | CH ₃ | C ₂ H ₅ | - |
| 886 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | CH ₃ | C ₂ H ₁₁ | - |
| 887 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 888 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 889 | CH ₃ | CH ₂ | H | Cl | CH ₃ | F | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 890 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 891 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 892 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 893 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | CH ₃ | c-C ₃ H ₇ | - |
| 894 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | CH ₃ | C ₂ H ₅ | - |
| 895 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | CH ₃ | C ₂ H ₅ | - |
| 896 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | CH ₃ | C ₂ H ₁₁ | - |
| 897 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 898 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 899 | CH ₃ | CH ₂ | H | Cl | CF ₃ | Cl | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 900 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | H | C ₂ H ₅ | oil |
| 901 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | 69-73 |
| 902 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | oil |
| 903 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 904 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 905 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 906 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | CH ₃ | c-C ₃ H ₇ | - |

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| 907 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | CH ₃ | C ₃ H ₇ | - |
| 908 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | CH ₃ | C ₄ H ₉ | - |
| 909 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | CH ₃ | C ₃ H ₁₁ | - |
| 910 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 911 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 912 | CH ₃ | CH ₂ | H | Cl | CF ₃ | F | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 913 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 914 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | c-C ₃ H ₅ | c-C ₃ H ₅ | oil |
| 915 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 916 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | CH ₃ | c-C ₃ H ₅ | - |
| 917 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | CH ₃ | C ₃ H ₇ | - |
| 918 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | CH ₃ | C ₄ H ₉ | - |
| 919 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | CH ₃ | C ₃ H ₁₁ | - |
| 920 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 921 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 922 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | Cl | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 923 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 924 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 925 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 926 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | CH ₃ | c-C ₃ H ₅ | - |
| 927 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | CH ₃ | C ₃ H ₇ | - |
| 928 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | CH ₃ | C ₄ H ₉ | - |
| 929 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | CH ₃ | C ₃ H ₁₁ | - |
| 930 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 931 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 932 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 933 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 934 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 150-151 |
| 935 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 936 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 937 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 938 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 939 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 940 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 941 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 942 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | CH ₃ | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 943 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 944 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 148-151 |
| 945 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | oil |
| 946 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |

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| 947 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | oil |
| 948 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 949 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 950 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 951 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | oil |
| 952 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | oil |
| 953 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 954 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 151-153 |
| 955 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 956 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | CH ₃ | c-C ₃ H ₅ | - |
| 957 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | CH ₃ | C ₃ H ₇ | - |
| 958 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | CH ₃ | C ₄ H ₉ | - |
| 959 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | CH ₃ | C ₃ H ₁₁ | - |
| 960 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 961 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 962 | CH ₃ | CH ₂ | H | Cl | H | Cl | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 963 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 964 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 965 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 966 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 967 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 968 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 969 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 970 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 971 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 972 | CH ₃ | CH ₂ | H | Cl | Cl | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 973 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 974 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 975 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 976 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 977 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 978 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 979 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 980 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 981 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 982 | CH ₃ | CH ₂ | H | Cl | CH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 983 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 984 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 985 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 986 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |

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| 987 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 988 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 989 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 990 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 991 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 992 | CH ₃ | CH ₂ | H | CH ₃ | Cl | OCH ₃ | H | C ₃ H ₅ | C ₂ H ₅ | - |
| 993 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 994 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 995 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 996 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 997 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 998 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 999 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 1000 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1001 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1002 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1003 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | oil |
| 1004 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 138-140 |
| 1005 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1006 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 1007 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 1008 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 1009 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 1010 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1011 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1012 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | oil |
| 1013 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1014 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1015 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1016 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 1017 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 1018 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 1019 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 1020 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1021 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1022 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1023 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | oil |
| 1024 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 119-120 |
| 1025 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₅ | 103-104 |
| 1026 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | CH ₃ | c-C ₃ H ₅ | - |

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| 1027 | CH ₃ | CH ₃ | H | Cl | OCF ₃ | H | H | CH ₃ | C ₃ H ₇ | oil |
| 1028 | CH ₃ | CH ₃ | H | Cl | OCF ₃ | H | H | CH ₃ | C ₄ H ₉ | oil |
| 1029 | CH ₃ | CH ₃ | H | Cl | OCF ₃ | H | H | CH ₃ | C ₃ H ₁₁ | - |
| 1030 | CH ₃ | CH ₃ | H | Cl | OCF ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1031 | CH ₃ | CH ₃ | H | Cl | OCF ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1032 | CH ₃ | CH ₃ | H | Cl | OCF ₃ | H | H | C ₂ H ₅ | C ₃ H ₇ | oil |
| 1033 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1034 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1035 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1036 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | CH ₃ | c-C ₃ H ₅ | - |
| 1037 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | CH ₃ | C ₃ H ₇ | - |
| 1038 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | CH ₃ | C ₄ H ₉ | - |
| 1039 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | CH ₃ | C ₃ H ₁₁ | - |
| 1040 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1041 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1042 | CH ₃ | CH ₃ | H | Cl | SCF ₃ | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 1044 | CH ₃ | CH ₃ | H | Cl | CF ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | 105-107 |
| 1045 | CH ₃ | CH ₃ | H | CF ₃ | Q3 | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 168-169 |
| 1046 | CH ₃ | CH ₃ | H | Cl | Q3 | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 130-132 |
| 1047 | CH ₃ | CH ₃ | H | CF ₃ | SCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1048 | CH ₃ | CH ₃ | H | Cl | SCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1049 | CH ₃ | CH ₃ | H | CF ₃ | COCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1050 | CH ₃ | CH ₃ | H | Cl | COCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1051 | CH ₃ | CH ₃ | H | CF ₃ | CHCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1052 | CH ₃ | CH ₃ | H | Cl | CHCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1053 | CH ₃ | CH ₃ | H | Cl | CH ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | 113-115 |
| 1054 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1055 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 128-130 |
| 1056 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1057 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | CH ₃ | c-C ₃ H ₅ | - |
| 1058 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | CH ₃ | C ₃ H ₇ | - |
| 1059 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | CH ₃ | C ₄ H ₉ | - |
| 1060 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | CH ₃ | C ₃ H ₁₁ | - |
| 1061 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1062 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1063 | CH ₃ | CH ₃ | H | OCH ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 1064 | CH ₃ | CH ₃ | H | OCH ₃ | CF ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1065 | CH ₃ | CH ₃ | H | OCH ₃ | CF ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 158-159 |
| 1066 | CH ₃ | CH ₃ | H | OCH ₃ | CF ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1067 | CH ₃ | CH ₃ | H | OCH ₃ | CF ₃ | H | H | CH ₃ | c-C ₃ H ₅ | - |

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| 1068 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | H | H | CH ₃ | C ₃ H ₇ | - |
| 1069 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | H | H | CH ₃ | C ₄ H ₉ | - |
| 1070 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | H | H | CH ₃ | C ₃ H ₁₁ | - |
| 1071 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1072 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1073 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1074 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | oil |
| 1075 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 129-130 |
| 1076 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₅ | 119-122 |
| 1077 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | CH ₃ | c-C ₃ H ₅ | - |
| 1078 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | CH ₃ | C ₃ H ₇ | oil |
| 1079 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | CH ₃ | C ₄ H ₉ | oil |
| 1080 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | CH ₃ | C ₃ H ₁₁ | - |
| 1081 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1082 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | oil |
| 1083 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | 77-78 |
| 1084 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1085 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1086 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1087 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 1088 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 1089 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 1090 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 1091 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1092 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1093 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1094 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1095 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1096 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1097 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 1098 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 1099 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 1100 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 1101 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1102 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1103 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1104 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1105 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1106 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1107 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |

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| 1108 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 1109 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 1110 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 1111 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1112 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1113 | CH ₃ | CH ₂ | H | OCH ₃ | CF ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1114 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1115 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1116 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1117 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 1118 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 1119 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 1120 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 1121 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1122 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1123 | CH ₃ | CH ₂ | H | OCH ₃ | CN | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1124 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1125 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1126 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1127 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | c-C ₃ H ₅ | - |
| 1128 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 1129 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | C ₄ H ₉ | - |
| 1130 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | C ₃ H ₁₁ | - |
| 1131 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 1132 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1133 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1134 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ OSO ₂ CH ₃ | 110-111 |
| 1135 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ SCH ₃ | 134-135 |
| 1136 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ Cl | 140-141 |
| 1137 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ CN | 142-147 |
| 1138 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ OSO ₂ CH ₃ | - |
| 1139 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₃ H ₇ | CH ₂ SCH ₃ | - |
| 1140 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ Cl | - |
| 1141 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ CN | - |
| 1142 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ OSO ₂ CH ₃ | - |
| 1143 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₃ H ₇ | CH ₂ SCH ₃ | - |
| 1144 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ Cl | - |
| 1145 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ CN | - |
| 1146 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ OSO ₂ CH ₃ | - |
| 1147 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ SCH ₃ | - |

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|------|-----------------|-----------------|---|-----------------|------------------|-----------------|-----------------|-----------------------------------|---------------------------------|---------|
| 1148 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ Cl | - |
| 1149 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ CN | - |
| 1150 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | C ₃ H ₇ | c-C ₃ H ₇ | oil |
| 1151 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | CH ₃ | C ₃ H ₇ | 97-98 |
| 1152 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₆ H ₅ | c-C ₃ H ₇ | - |
| 1153 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₆ H ₅ | c-C ₃ H ₇ | oil |
| 1154 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₆ H ₅ | c-C ₃ H ₇ | - |
| 1155 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | C ₆ H ₅ | c-C ₃ H ₇ | oil |
| 1156 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₆ H ₅ | c-C ₃ H ₇ | 119-120 |
| 1157 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | C ₆ H ₅ | c-C ₃ H ₇ | oil |
| 1158 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | C ₆ H ₅ | c-C ₃ H ₇ | oil |
| 1159 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₆ H ₅ | c-C ₃ H ₇ | - |
| 1160 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₆ H ₅ | c-C ₃ H ₇ | - |
| 1161 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | oil |
| 1162 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | - |
| 1163 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | oil |
| 1164 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | - |
| 1165 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | - |
| 1166 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | - |
| 1167 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | - |
| 1168 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | - |
| 1169 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | - |
| 1170 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | 4-F-C ₆ H ₄ | c-C ₃ H ₇ | - |
| 1171 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | c-C ₄ H ₉ | 109-110 |
| 1172 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | c-C ₄ H ₉ | - |
| 1173 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | CH ₃ | c-C ₄ H ₉ | 136-137 |
| 1174 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | CH ₃ | c-C ₄ H ₉ | - |
| 1175 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | CH ₃ | c-C ₄ H ₉ | - |
| 1176 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | CH ₃ | c-C ₄ H ₉ | - |
| 1177 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | CH ₃ | c-C ₄ H ₉ | - |
| 1178 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | CH ₃ | c-C ₄ H ₉ | - |
| 1179 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | CH ₃ | c-C ₄ H ₉ | - |
| 1180 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | CH ₃ | c-C ₄ H ₉ | - |
| 1181 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₃ H ₇ | c-C ₄ H ₉ | - |
| 1182 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | c-C ₄ H ₉ | - |
| 1183 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₃ H ₇ | c-C ₄ H ₉ | - |
| 1184 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₃ H ₇ | c-C ₄ H ₉ | - |
| 1185 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | C ₃ H ₇ | c-C ₄ H ₉ | - |
| 1186 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₃ H ₇ | c-C ₄ H ₉ | - |
| 1187 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | C ₃ H ₇ | c-C ₄ H ₉ | - |

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| 1188 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1189 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1190 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1191 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1192 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1193 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1194 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1195 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1196 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1197 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1198 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1199 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1200 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | C ₂ H ₅ | c-C ₄ H ₉ | - |
| 1201 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1202 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1203 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1204 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1205 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1206 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1207 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1208 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1209 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1210 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | c-C ₄ H ₉ | c-C ₄ H ₉ | - |
| 1211 | CH ₃ | S | H | SCH ₃ | Cl | H | Cl | C ₂ H ₅ | C ₂ H ₅ | 63-65 |
| 1212 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | 152-154 |
| 1213 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 1214 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 1215 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | CH ₃ | c-C ₄ H ₉ | - |
| 1216 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | CH ₃ | C ₂ H ₅ | - |
| 1217 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1218 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1219 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1220 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | CH ₃ | C ₂ H ₅ | - |
| 1221 | CH ₃ | CH ₂ | H | OCH ₃ | Cl | H | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1222 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | c-C ₃ H ₇ | c-C ₃ H ₇ | oil |
| 1223 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 1224 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 1225 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | CH ₃ | c-C ₄ H ₉ | - |
| 1226 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | CH ₃ | C ₂ H ₅ | - |
| 1227 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | - |

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| 1228 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1229 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1230 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | CH ₃ | C ₄ H ₉ | - |
| 1231 | CH ₃ | CH ₂ | H | OCH ₃ | CH ₃ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1232 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | c-C ₃ H ₅ | c-C ₃ H ₅ | 176-178 |
| 1233 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1234 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 1235 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | CH ₃ | c-C ₄ H ₇ | - |
| 1236 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | CH ₃ | C ₃ H ₇ | - |
| 1237 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | C ₂ H ₅ | C ₃ H ₇ | - |
| 1238 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | C ₃ H ₅ | C ₃ H ₅ | - |
| 1239 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | C ₃ H ₇ | C ₃ H ₇ | - |
| 1240 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | CH ₃ | C ₄ H ₉ | - |
| 1241 | CH ₃ | CH ₂ | H | OCH ₃ | OCH ₃ | H | F | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1242 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1243 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1244 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | C ₃ H ₇ | c-C ₃ H ₅ | 115-118 |
| 1245 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | CH ₃ | c-C ₄ H ₇ | - |
| 1246 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | CH ₃ | C ₃ H ₇ | - |
| 1247 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 1248 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | C ₂ H ₅ | C ₃ H ₅ | - |
| 1249 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1250 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | CH ₃ | C ₄ H ₉ | - |
| 1251 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | H | 4-CH ₃ O-C ₆ H ₄ | 57-70 |
| 1252 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | BnOCH ₂ | BnOCH ₂ | oil |
| 1253 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | CH ₃ | C ₄ H ₉ | 119-120 |
| 1254 | CH ₃ | CH ₂ | H | CF ₃ | F | H | H | C ₄ H ₉ | C ₄ H ₉ | 135-139 |
| 1255 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | C ₃ H ₇ | c-C ₃ H ₅ | oil |
| 1256 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | C ₃ H ₅ | C ₃ H ₇ | oil |
| 1257 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | H | CH ₂ =CH-CH=CH | 83-85 |
| 1258 | CH ₃ | CH ₂ | H | CF ₃ | OBn | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 163-165 |
| 1259 | CH ₃ | CH ₂ | H | CF ₃ | OH | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 245-246 |
| 1260 | CH ₃ | CH ₂ | H | CF ₃ | OC ₃ H ₇ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 127-128 |
| 1261 | CH ₃ | CH ₂ | H | CF ₃ | OC ₃ H ₇ | H | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1262 | CH ₃ | CH ₂ | H | CF ₃ | OC ₃ H ₇ | H | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 1263 | CH ₃ | CH ₂ | H | CF ₃ | OC ₃ H ₇ | H | H | CH ₃ | c-C ₄ H ₇ | - |
| 1264 | CH ₃ | CH ₂ | H | CF ₃ | OC ₃ H ₇ | H | H | CH ₃ | C ₃ H ₇ | - |
| 1265 | CH ₃ | CH ₂ | H | CF ₃ | OC ₃ H ₇ | H | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 1266 | CH ₃ | CH ₂ | H | CF ₃ | OC ₃ H ₇ | H | H | C ₂ H ₅ | C ₃ H ₅ | - |
| 1267 | CH ₃ | CH ₂ | H | CF ₃ | OC ₃ H ₇ | H | H | C ₃ H ₇ | C ₃ H ₇ | - |

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| 1268 | CH ₃ | CH ₂ | H | CF ₃ | OC ₂ H ₅ | H | H | CH ₃ | C ₄ H ₉ | - |
| 1269 | CH ₃ | CH ₂ | H | CF ₃ | OC ₂ H ₅ | H | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1284 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1285 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 1286 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 1287 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | CH ₃ | c-C ₄ H ₉ | - |
| 1288 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | CH ₃ | C ₃ H ₇ | - |
| 1289 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 1290 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1291 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1292 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | CH ₃ | C ₄ H ₉ | - |
| 1293 | CH ₃ | CH ₂ | H | CH ₃ | OH | F | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1294 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | CH ₃ | 101-102 |
| 1295 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | OCH ₃ | H | CH ₃ | C ₂ H ₅ | oil |
| 1296 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₂ H ₅ | 4-CH ₃ O-C ₆ H ₄ | oil |
| 1297 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | C ₂ H ₅ | C ₂ H ₅ | 133-135 |
| 1298 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | 123-125 |
| 1299 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | C ₃ H ₇ | C ₃ H ₇ | 125-127 |
| 1300 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | 157-159 |
| 1301 | CH ₃ | O | H | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1302 | CH ₃ | O | H | Cl | CF ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 149-150 |
| 1303 | CH ₃ | O | H | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 124-125 |
| 1304 | CH ₃ | O | H | Cl | OCF ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1305 | CH ₃ | O | H | Cl | CH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1306 | CH ₃ | O | H | CF ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1307 | CH ₃ | O | H | Cl | Cl | H | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1308 | CH ₃ | O | H | CH ₃ | OCH ₃ | Cl | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1309 | CH ₃ | O | H | CH ₃ | OCH ₃ | F | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1310 | CH ₃ | O | H | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | - |
| 1311 | CH ₃ | O | H | Cl | CF ₃ | H | H | CH ₃ | C ₃ H ₇ | - |
| 1312 | CH ₃ | O | H | Cl | OCH ₃ | H | H | CH ₃ | C ₃ H ₇ | - |
| 1313 | CH ₃ | O | H | Cl | OCF ₃ | H | H | CH ₃ | C ₃ H ₇ | - |
| 1314 | CH ₃ | O | H | Cl | CH ₃ | H | H | CH ₃ | C ₃ H ₇ | - |
| 1315 | CH ₃ | O | H | CF ₃ | OCH ₃ | H | H | CH ₃ | C ₃ H ₇ | - |
| 1316 | CH ₃ | O | H | Cl | Cl | H | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 1317 | CH ₃ | O | H | CH ₃ | OCH ₃ | Cl | H | CH ₃ | C ₃ H ₇ | - |
| 1318 | CH ₃ | O | H | CH ₃ | OCH ₃ | F | H | CH ₃ | C ₃ H ₇ | - |
| 1319 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₆ H ₅ | C ₆ H ₅ | oil |
| 1320 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₆ H ₅ | CH ₃ | oil |
| 1321 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | c-C ₃ H ₅ | 2-CH ₃ -C ₆ H ₄ | oil |

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| 1322 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₆ H ₅ | CH(CH ₂ OH) ₂ | oil |
| 1323 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₆ H ₅ | CO ₂ C ₆ H ₅ | oil |
| 1324 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₆ H ₅ | CO ₂ H | oil |
| 1325 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₆ H ₅ | CH ₂ OH | oil |
| 1326 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 2-Cl-C ₆ H ₄ | oil |
| 1327 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 3-Cl-C ₆ H ₄ | oil |
| 1328 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 4-Cl-C ₆ H ₄ | oil |
| 1329 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 3-CH ₂ O-C ₆ H ₄ | oil |
| 1330 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 3-CN-C ₆ H ₄ | oil |
| 1331 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 4-CN-C ₆ H ₄ | oil |
| 1332 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 4-BnO-C ₆ H ₄ | oil |
| 1333 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 2,5-(CH ₂ O)- C ₆ H ₃ | oil |
| 1334 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | H | 2-CH ₂ O-C ₆ H ₄ | oil |
| 1335 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CN | c-C ₆ H ₃ | oil |
| 1336 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | CH ₂ OC ₂ H ₅ | 96-97 |
| 1337 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | CH(OH)CH ₂ OC ₂ H ₅ | oil |
| 1338 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | CH(OH)CH ₂ C ₆ H ₅ | oil |
| 1339 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | CH(OH)C ₆ H ₅ | oil |
| 1340 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH(CH ₃) ₂ | C(O)-1- morpholinyl | 154-155 |
| 1341 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | C ₆ H ₅ | CO ₂ CH ₃ | oil |
| 1342 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | CO ₂ CH ₃ | oil |
| 1343 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | CN | oil |
| 1344 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | COCH ₃ | oil |
| 1345 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 2-Cl-C ₆ H ₄ | 149-152 |
| 1346 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 3-Cl-C ₆ H ₄ | oil |
| 1347 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 4-F-C ₆ H ₄ | 148-149 |
| 1348 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 4-CN-C ₆ H ₄ | 199-200 |
| 1349 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | H | 4-Cl-C ₆ H ₄ | 183-184 |
| 1350 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | c-C ₆ H ₅ | c-C ₆ H ₅ | - |
| 1351 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₆ H ₅ | c-C ₆ H ₅ | - |
| 1352 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | c-C ₆ H ₅ | c-C ₆ H ₅ | - |
| 1353 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | c-C ₆ H ₅ | c-C ₆ H ₅ | - |
| 1354 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | c-C ₆ H ₅ | c-C ₆ H ₅ | - |
| 1355 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | c-C ₆ H ₅ | c-C ₆ H ₅ | - |
| 1356 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | c-C ₆ H ₅ | c-C ₆ H ₅ | - |
| 1357 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | c-C ₆ H ₅ | c-C ₆ H ₅ | - |
| 1358 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | c-C ₆ H ₅ | c-C ₆ H ₅ | - |
| 1359 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | F | H | c-C ₆ H ₅ | c-C ₆ H ₅ | - |

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|------|-----------------|-----------------|---|-----------------|------------------|-----------------|-----------------|---------------------------------|--|-----|
| 1360 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | c-C ₃ H ₇ | c-C ₃ H ₇ | - |
| 1361 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₂ H ₅ | c-C ₃ H ₇ | - |
| 1362 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₃ H ₇ | c-C ₃ H ₇ | - |
| 1363 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | CH ₃ | c-C ₄ H ₉ | - |
| 1364 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | CH ₃ | C ₃ H ₇ | - |
| 1365 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 1366 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₂ H ₅ | C ₂ H ₅ | - |
| 1367 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 1368 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | CH ₃ | C ₄ H ₉ | - |
| 1369 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | F | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 1370 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | C ₂ H ₅ | C ₃ H ₇ | oil |
| 1371 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | oil |
| 1372 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | - |
| 1373 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | - |
| 1374 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | - |
| 1375 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | - |
| 1376 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | - |
| 1377 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | - |
| 1378 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | - |
| 1379 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | - |
| 1380 | CH ₃ | O | H | Cl | Cl | H | H | CH ₃ | 2-CH ₃ -c-C ₃ H ₇ | - |
| 1381 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1382 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1383 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1384 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1385 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1386 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1387 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1388 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1389 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1390 | CH ₃ | O | H | Cl | Cl | H | H | CH ₃ | 2-C ₆ H ₅ -c-C ₃ H ₇ | - |
| 1391 | CH ₃ | CH ₂ | H | Cl | Cl | H | H | CH ₃ | 2-(2-pyridyl)-c-C ₃ H ₇ | - |
| 1392 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | 2-(2-pyridyl)-c-C ₃ H ₇ | - |
| 1393 | CH ₃ | CH ₂ | H | Cl | CF ₃ | H | H | CH ₃ | 2-(2-pyridyl)-c-C ₃ H ₇ | - |
| 1394 | CH ₃ | CH ₂ | H | Cl | OCH ₃ | H | H | CH ₃ | 2-(2-pyridyl)-c-C ₃ H ₇ | - |

| | | | | | | | | | | |
|------|-----------------|-----------------|---|-----------------|------------------|----|-----------------|-----------------|---|---|
| 1395 | CH ₃ | CH ₂ | H | Cl | OCF ₃ | H | H | CH ₃ | 2-(2-pyridyl)- c-C ₃ H ₄ | - |
| 1396 | CH ₃ | CH ₂ | H | Cl | CH ₃ | H | H | CH ₃ | 2-(2-pyridyl)- c-C ₃ H ₄ | - |
| 1397 | CH ₃ | CH ₂ | H | CF ₃ | OCH ₃ | H | H | CH ₃ | 2-(2-pyridyl)- c-C ₃ H ₄ | - |
| 1398 | CH ₃ | CH ₂ | H | Cl | Cl | H | CH ₃ | CH ₃ | 2-(2-pyridyl)- c-C ₃ H ₄ | - |
| 1399 | CH ₃ | CH ₂ | H | CH ₃ | OCH ₃ | Cl | H | CH ₃ | 2-(2-pyridyl)- c-C ₃ H ₄ | - |
| 1400 | CH ₃ | O | H | Cl | Cl | H | H | CH ₃ | 2-(2-pyridyl)- c-C ₃ H ₄ | - |

Key:

(a) Where the compound is indicated as an "oil", data is provided below:

- Example 3 spectral data: TLC R_f 0.27 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.90 (1H, s), 6.95 (2H, s), 4.45 (1H, br), 4.27-4.17 (2H, m), 3.85 (1H, dd, J = 9.5, 4.8 Hz), 3.27 (3H, s), 2.94 (2H, q, J = 7.5 Hz), 2.56-2.46 (1H, m), 2.32 (3H, s), 2.06 (3H, s), 2.03 (3H, s), 1.37 (3H, t, J = 7.5 Hz), 0.85 (3H, t, J = 7.5 Hz). MS (NH₃-CI): m/e 355 (3), 354 (25), 353 (100). Analysis calc'd for C₂₁H₂₂N₄O·1.5H₂O: C, 66.46; H, 8.23; N, 14.76; found: C, 67.00; H, 8.10; N, 14.38.
- 10 Example 8 spectral data: TLC R_f 0.34 (50:50 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.89 (1H, s), 6.95 (2H, s), 4.46 (1H, br), 3.41-3.33 (1H, m), 3.22 (3H, s), 2.94 (2H, q, J = 7.3 Hz), 2.93-2.85 (1H, m), 2.84-2.69 (2H, m), 2.51 (1H, br), 2.32 (3H, s), 2.30-2.20 (1H, m), 2.04 (6H, s), 1.37 (3H, t, J = 7.7 Hz), 0.84 (3H, t, J = 7.3 Hz). MS (NH₃-CI): m/e calc'd for C₂₂H₂₀N₄O: 366.2420, found 366.2400; 369 (3), 368 (27), 367 (100).
- 15 Example 10 spectral data: TLC R_f 0.13 (ethyl acetate). ¹H NMR (300 MHz, CDCl₃): δ 8.93 (1H, s), 8.10 (1H, s), 7.96 (1H, s), 6.96 (2H, s), 4.39 (1H, br), 4.24-4.14 (1H, m), 4.12-4.00 (1H, m), 3.20 (1H, br), 2.80 (2H, q, J = 7.0 Hz), 2.78-2.68 (1H, m), 2.42 (1H, br), 2.33 (3H, s), 2.13-2.04 (1H, m), 2.06 (3H, s), 2.03 (3H, s), 1.33 (3H, t, J = 7.5 Hz), 0.80 (3H, t, J = 7.3 Hz). MS (NH₃-CI): m/e calc'd for C₂₃H₂₀N₄: 404.2563, found 404.2556; 406 (4), 405 (28), 404 (100).
- 20 Example 11 spectral data: TLC R_f 0.60 (ethyl acetate). ¹H NMR (300 MHz, CDCl₃): δ 8.92 (1H, s), 8.51 (1H, s), 6.96 (2H, s), 4.78-4.68 (1H, m), 4.57-4.47 (1H, m), 4.32-4.22 (1H, m), 3.43 (1H, br), 2.81 (2H, q, J = 6.9 Hz), 2.78 (1H, br), 2.43 (1H, br), 2.33 (3H, s), 2.10-2.00 (1H, m), 2.07 (3H, s), 2.03 (3H, s), 1.32 (3H, t, J = 7.0 Hz), 0.78
- 25

(3H, t, J = 7.5 Hz). MS (NH₃-CI): m/e calc'd for C₂₂H₂₃N₃: 405.2515, found 405.2509; 407 (4), 406 (27), 405 (100).

Example 18 spectral data: TLC R_f 0.20 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.00 (1H, s), 7.26 (1H, obscured), 6.96 (2H, s), 6.86-6.76 (3H, m), 5.46

5 (2H, s), 3.76 (3H, s), 2.85 (2H, q, J = 7.7 Hz), 2.33 (3H, s), 2.06 (6H, s), 1.28 (3H, t, J = 7.7 Hz). MS (NH₃-CI): m/e 389 (4), 388 (28), 387 (100). Analysis calc'd for C₂₄H₂₅N₃O: C, 74.58; H, 6.78; N, 14.50; found: C, 74.36; H, 6.73; N, 13.83.

Example 27 spectral data: TLC R_f 0.20 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.96 (1H, s), 6.95 (2H, s), 4.25 (2H, t, J = 7.5 Hz), 2.93 (2H, q, J = 7.7

10 Hz), 2.32 (3H, s), 2.04 (6H, s), 1.91-1.86 (2H, m), 1.50-1.38 (2H, m), 1.39 (3H, t, J = 7.7 Hz), 1.01 (3H, t, J = 7.5 Hz). MS (NH₃-CI): m/e 325 (3), 324 (23), 323 (100).

Example 28 spectral data: TLC R_f 0.28 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.96 (1H, s), 6.95 (2H, s), 4.24 (2H, t, J = 7.9 Hz), 2.93 (2H, q, J = 7.6

15 Hz), 2.32 (3H, s), 2.04 (6H, s), 1.90 (2H, m), 1.44-1.36 (7H, m), 0.93 (3H, t, J = 7.1 Hz). MS (NH₃-CI): m/e 339 (3), 338 (25), 337 (100). Analysis calc'd for C₂₁H₂₃N₃: C, 74.96; H, 8.40; N, 16.65; found: C, 74.24; H, 8.22; N, 16.25.

Example 34 spectral data: MS (ESI): m/e 365 (M+2), 363 (M+H⁺, 100%).

Example 35 spectral data: TLC R_f 0.31 (20:80 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.94 (1H, s), 7.71 (1H, d, J = 8.4 Hz), 7.58 (1H, d, J = 1.8 Hz), 7.41

20 (1H, dd, J = 8.4, 1.8 Hz), 4.27 (1H, br), 2.95 (2H, q, J = 7.3 Hz), 2.41 (2H, br), 2.11-1.98 (2H, br), 1.42 (3H, t, J = 7.3 Hz), 1.37-1.20 (3H, m), 1.09-0.99 (1H, m), 0.84 (3H, t, J = 7.7 Hz), 0.82 (3H, t, J = 7.7 Hz). MS (NH₃-CI): m/e calc'd for C₂₀H₂₃N₃Cl₂: 391.1456, found 391.1458; 395 (11), 394 (14), 393 (71), 392 (29), 391 (100).

25 Example 38 spectral data: MS (NH₃-CI): m/e 375 (M+H⁺, 100%).

Example 40 spectral data: MS (NH₃-CI): m/e 377 (M+H⁺, 100%).

Example 48 spectral data: MS (NH₃-CI): m/e 423 (M+H⁺, 100%).

Example 50 spectral data: TLC R_f 0.27 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.03 (1H, s), 7.70 (1H, d, J = 8.0 Hz), 7.59 (1H, d, J = 1.8 Hz), 7.41

30 (1H, dd, J = 8.0, 1.8 Hz), 7.36-7.30 (2H, m), 7.24-7.19 (3H, m), 5.50 (2H, s), 2.87 (2H, q, J = 7.5 Hz), 1.31 (3H, t, J = 7.5 Hz). MS (NH₃-CI): m/e calc'd for C₂₀H₁₆N₄Cl₂: 382.0752, found 382.0746; 388 (3), 387 (12), 386 (16), 385 (66), 384 (26), 383 (100).

Example 51 spectral data: MS (NH₃-CI): m/e 413 (M+H⁺, 100%).

35 Example 54 spectral data: MS (NH₃-CI): m/e 459 (M+H⁺, 100%).

Example 68 spectral data: TLC R_f 0.28 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.91 (1H, s), 6.69 (2H, s), 4.30-4.19 (1H, m), 3.82 (3H, s), 2.92 (2H, q, J = 7.6 Hz), 2.41 (1H, br), 2.08 (3H, s), 2.07 (3H, s), 2.06 (1H, br), 1.38 (3H, t, J = 7.6 Hz), 1.36-1.22 (4H, m), 1.10-0.98 (1H, m), 0.96-0.87 (1H, m), 0.84 (3H, t,

$J = 7.0$ Hz), 0.81 (3H, t, $J = 6.7$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 383 (4), 382 (27), 381 (100).

Example 122 spectral data: TLC R_f 0.10 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.97 (1H, s), 6.94 (2H, s), 4.14 (2H, d, $J = 7.7$ Hz), 3.48 (1H, q, $J = 7.0$ Hz), 2.63 (3H, s), 2.31 (3H, s), 2.01 (6H, s), 1.43-1.19 (8H, m), 0.94 (3H, t, $J = 7.3$ Hz), 0.84 (3H, t, $J = 7.0$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 367 (3), 366 (25), 365 (100).

Example 123 spectral data: TLC R_f 0.24 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.97 (1H, s), 6.94 (2H, s), 4.25 (2H, t, $J = 8.1$ Hz), 3.48 (1H, q, $J = 7.1$ Hz), 2.63 (3H, s), 2.31 (3H, s), 2.01 (6H, s), 1.81 (2H, m), 1.47-1.19 (8H, m), 0.91 (6H, m). MS ($\text{NH}_3\text{-CI}$): m/e 381 (4), 380 (27), 379 (100). Analysis calc'd for $\text{C}_{24}\text{H}_{24}\text{N}_4$: C, 76.15; H, 9.05; N, 14.80; found: C, 76.29; H, 9.09; N, 14.75.

Example 202 spectral data: TLC R_f 0.20 (10:90 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.82 (1H, s), 6.96 (2H, s), 4.46-4.38 (1H, m), 4.13 (3H, s), 2.34 (3H, s), 2.28-2.11 (2H, m), 2.07 (6H, s), 1.95-1.81 (2H, m), 1.38-1.17 (3H, m), 1.14-0.99 (1H, m), 0.83 (3H, t, $J = 7.7$ Hz), 0.80 (3H, t, $J = 7.7$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{22}\text{H}_{20}\text{N}_4\text{O}$: 366.2420, found 366.2408; 369 (4), 368 (26), 367 (100).

Example 404 spectral data: TLC R_f 0.20 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 6.93 (2H, s), 4.20 (2H, t, $J = 7.7$ Hz), 2.90 (2H, q, $J = 7.6$ Hz), 2.83 (3H, s), 2.30 (3H, s), 2.03 (6H, s), 1.88 (2H, m), 1.42-1.34 (7H, m), 0.93 (3H, t, $J = 6$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 353 (3), 352 (27), 351 (100).

Example 414 spectral data: TLC R_f 0.36 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.92 (1H, s), 7.66 (1H, d, $J = 8.1$ Hz), 7.32-7.26 (2H, m), 4.54 (1H, m), 2.95 (2H, q, $J = 7.4$ Hz), 2.43 (3H, s), 2.39 (1H, m), 2.03 (1H, m), 1.74 (3H, d, $J = 7.0$ Hz), 1.41 (3H, t, $J = 7.5$ Hz), 1.31 (1H, m), 1.16 (1H, m), 0.92 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{19}\text{H}_{24}\text{N}_4\text{Cl}$: 343.1690, found 343.1704; 346 (7), 345 (34), 344 (23), 343 (100).

Example 415 spectral data: TLC R_f 0.25 (10:90 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.91 (1H, s), 7.71 (1H, d, $J = 8.1$ Hz), 7.34-7.30 (2H, m), 4.30-4.20 (1H, m), 2.94 (2H, q, $J = 7.5$ Hz), 2.50-2.35 (2H, m), 2.44 (3H, s), 2.08-1.95 (2H, m), 1.43 (3H, t, $J = 7.5$ Hz), 1.29 (3H, m), 1.08-0.98 (1H, m), 0.84 (3H, t, $J = 7.0$ Hz), 0.81 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 374 (7), 373 (33), 372 (25), 371 (100). Analysis calc'd for $\text{C}_{21}\text{H}_{22}\text{ClN}_4$: C, 68.00; H, 7.35; N, 15.10; found: C, 68.25; H, 7.30; N, 14.85.

Example 424 spectral data: TLC R_f 0.28 (5:95 ethyl acetate-dichloromethane). ^1H NMR (300 MHz, CDCl_3): δ 8.95 (1H, s), 7.60 (1H, d, $J = 7.7$ Hz), 7.37 (1H, d, $J = 0.8$ Hz), 7.21 (1H, dd, $J = 7.7, 0.8$ Hz), 4.58-4.50 (1H, m), 2.96 (2H, dq, $J = 7.5, 2.0$ Hz), 2.46-2.33 (1H, m), 2.40 (3H, s), 2.08-1.96 (1H, m), 1.74 (3H, d, $J = 6.6$ Hz), 1.40 (3H, t, $J = 7.5$ Hz), 1.39-1.22 (1H, m), 1.20-1.08 (1H, m), 0.92 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$):

m/e calc'd for $C_{11}H_{21}ClN_4$: 343.1690, found 343.1697; 346 (8), 345 (38), 344 (25), 343 (100).

Example 434 spectral data: TLC R_f 0.78 (50:50 ethyl acetate-hexane). 1H NMR (300 MHz, $CDCl_3$): δ 8.90 (1H, s), 6.95 (2H, s), 2.97 (2H, J = 7.3 Hz), 2.60-2.50 (1H, m), 2.41-2.33 (1H, m), 2.32 (3H, s), 2.20-2.10 (1H, m), 2.05 (3H, s), 2.02 (3H, s), 1.85-1.80 (1H, m), 1.39 (3H, t, J = 7.5 Hz), 0.85 (3H, t, J = 7.5 Hz), 0.50-0.35 (2H, m), 0.25-0.15 (1H, m), 0.10-0.00 (1H, m). MS (NH_3 -CI): m/e calc'd for $C_{22}H_{36}N_4$: 362.2470, found 362.2458; 365 (4), 364 (27), 363 (100).

Example 436 spectral data: TLC R_f 0.31 (30:70 ethyl acetate-hexane). 1H NMR (300 MHz, $CDCl_3$): δ 8.88 (1H, s), 7.77 (1H, d, J = 9.2 Hz), 6.87 (2H, m), 4.40-4.25 (1H, m), 3.86 (3H, s), 2.99 (2H, q, J = 7.5 Hz), 2.60-2.35 (2H, m), 2.47 (3H, s), 2.15-2.00 (1H, m), 1.80-1.70 (1H, m), 1.45 (3H, t, J = 7.5 Hz), 0.84 (3H, t, J = 7.5 Hz), 0.50-0.35 (2H, m), 0.30-0.20 (1H, m), 0.10-0.00 (1H, m), -0.85 - -0.95 (1H, m).

Example 437 spectral data: TLC R_f 0.25 (30:70 ethyl acetate-hexane). 1H NMR (300 MHz, $CDCl_3$): δ 8.90 (1H, s), 7.73 (1H, d, J = 9.2 Hz), 6.89-6.86 (2H, m), 4.58-4.51 (1H, m), 3.86 (3H, s), 2.95 (2H, dq, J = 7.6, 1.8 Hz), 2.47 (3H, s), 2.45-2.34 (1H, m), 2.07-1.97 (1H, m), 1.73 (3H, d, J = 7.0 Hz), 1.42 (3H, t, J = 7.6 Hz), 1.40-1.27 (1H, m), 1.20-1.07 (1H, m), 0.92 (3H, t, J = 7.4 Hz). MS (NH_3 -CI): m/e calc'd for $C_{20}H_{28}N_4O$: 339.2185, found 339.2187; 341 (3), 340 (22), 339 (100). Analysis calc'd for $C_{20}H_{28}N_4O$: C, 70.98; H, 7.74; N, 16.55; found: C, 69.97; H, 7.48; N, 15.84.

Example 438 spectral data: TLC R_f 0.42 (40:60 ethyl acetate-hexane). 1H NMR (300 MHz, $CDCl_3$): δ 8.98 (1H, s), 7.77 (1H, d, J = 9.1 Hz), 7.17 (2H, d, J = 8.8 Hz), 6.90-6.83 (4H, m), 5.42 (2H, s), 3.86 (3H, s), 3.78 (3H, s), 2.86 (2H, q, J = 7.5 Hz), 2.49 (3H, s), 1.33 (3H, t, J = 7.5 Hz). MS (NH_3 -CI): m/e 391 (4), 390 (26), 389 (100). Analysis calc'd for $C_{23}H_{34}N_4O_2$: C, 71.11; H, 6.24; N, 14.42; found: C, 71.14; H, 5.97; N, 14.03.

Example 439 spectral data: TLC R_f 0.41 (30:70 ethyl acetate-hexane). 1H NMR (300 MHz, $CDCl_3$): δ 8.89 (1H, s), 7.77 (1H, d, J = 3.1 Hz), 6.89 (2H, m), 3.86 (3H, s), 3.53 (1H, m), 2.91 (2H, q, J = 7.5 Hz), 2.49 (3H, s), 2.28 (1H, m), 2.21 (1H, m), 1.43 (3H, t, J = 7.3 Hz), 0.86 (3H, t, J = 7.3 Hz), 0.78 (2H, m), 0.46 (2H, m), 0.20 (1H, m).

Example 440 spectral data: TLC R_f 0.28 (30:70 ethyl acetate-hexane). 1H NMR (300 MHz, $CDCl_3$): δ 8.89 (1H, s), 7.73 (1H, d, J = 9.1 Hz), 6.90-6.86 (2H, m), 4.60-4.40 (1H, m), 3.86 (3H, s), 2.95 (2H, dq, J = 7.7, 2.2 Hz), 2.47 (3H, s), 2.44-2.36 (1H, m), 2.05-1.98 (1H, m), 1.74 (3H, d, J = 7.0 Hz), 1.42 (3H, t, J = 7.5 Hz), 1.40-1.20 (5H, m), 1.13-1.05 (1H, m), 0.830 (3H, t, J = 6.6 Hz).

Example 502 spectral data: TLC R_f 0.63 (50:50 ethyl acetate-hexane). 1H NMR (300 MHz, $CDCl_3$): δ 8.92 (1H, s), 6.95 (2H, s), 4.60-4.47 (1H, m), 2.93 (2H, q, J = 7.7 Hz), 2.43-2.33 (1H, m), 2.32 (3H, s), 2.16-2.06 (1H, m), 2.05 (3H, s), 2.03 (3H, s), 1.76 (3H, d, J = 7.0 Hz), 1.36 (3H, t, J = 7.7 Hz), 1.36-1.20 (4H, m), 0.86 (3H, t, J = 7.2

Hz). MS (NH₃-CI): *m/e* calc'd for C₂₂H₂₀N₄: 350.2470, found 350.2480; 353 (3), 352 (28), 351 (100).

5 Example 503 spectral data: ¹H NMR (300 MHz, CDCl₃): δ 8.92 (1H, s), 6.94 (2H, s), 4.58-4.48 (1H, m), 2.93 (2H, q, *J* = 7.3 Hz), 2.32 (3H, s), 2.05 (3H, s), 2.02 (3H, s), 1.76 (3H, d, *J* = 6.6 Hz), 1.36 (3H, t, *J* = 7.3 Hz), 1.34-1.05 (8H, m), 0.88 (3H, t, *J* = 7 Hz). MS (NH₃-CI): *m/e* calc'd for C₂₅H₂₂N₄: 365.2705, found 365.2685; 367 (3), 366 (27), 365 (100).

10 Example 506 spectral data: TLC R_f 0.28 (20:80 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.95 (1H, s), 7.67 (1H, d, *J* = 8.4 Hz), 7.57 (1H, d, *J* = 1.8 Hz), 7.42-7.37 (1H, m), 4.56 (1H, hextet, *J* = 7.1 Hz), 2.99 (2H, q, *J* = 7.5 Hz), 2.43-2.33 (1H, m), 2.09-1.97 (1H, m), 1.74 (3H, d, *J* = 7.0 Hz), 1.41 (3H, t, *J* = 7.5 Hz), 1.35-1.07 (2H, m), 0.92 (3H, t, *J* = 7.3 Hz). MS (NH₃-CI): *m/e* 367 (12), 366 (14), 365 (67), 364 (24), 363 (100).

15 Example 507 spectral data: MS (NH₃-CI): *m/e* 377 (M+H⁺, 100%).
Example 511 spectral data: TLC R_f 0.51 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.97 (1H, s), 7.87 (1H, d, *J* = 8.1 Hz), 7.83 (1H, d, *J* = 1.1 Hz), 7.68 (1H, dd, *J* = 8.1, 1.1 Hz), 3.60-3.51 (1H, m), 2.94 (2H, q, *J* = 7.5 Hz), 2.53-2.39 (1H, m), 2.36-2.20 (1H, m), 1.96 (1H, br), 1.42 (3H, t, *J* = 7.5 Hz), 0.88 (3H, t, *J* = 7.3 Hz), 0.88-0.78 (1H, m), 0.52-0.44 (2H, m), 0.24-0.16 (1H, m). MS (NH₃-CI): *m/e* 412 (7), 411 (33), 410 (23), 409 (100).

20 Example 513 spectral data: TLC R_f 0.62 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.97 (1H, s), 7.87 (1H, d, *J* = 8.0 Hz), 7.83 (1H, d, *J* = 0.7 Hz), 7.68 (1H, dd, *J* = 8.0, 0.7 Hz), 4.21 (1H, br), 2.96 (2H, q, *J* = 7.5 Hz), 2.42 (2H, br), 2.12-1.97 (2H, m), 1.43 (3H, t, *J* = 7.5 Hz), 1.40-1.20 (4H, m), 0.85 (3H, t, *J* = 7.3 Hz), 0.83 (3H, t, *J* = 7.6 Hz). MS (NH₃-CI): *m/e* 428 (8), 427 (38), 426 (29), 425 (100).

25 Example 514 spectral data: TLC R_f 0.51 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.96 (1H, s), 7.86 (1H, d, *J* = 8.1 Hz), 7.83 (1H, d, *J* = 0.8 Hz), 7.68 (1H, dd, *J* = 8.1, 0.8 Hz), 4.20 (1H, br), 2.97 (2H, q, *J* = 7.7 Hz), 2.54-2.39 (2H, m), 2.15-2.01 (2H, m), 1.43 (3H, t, *J* = 7.7 Hz), 0.84 (6H, t, *J* = 7.5 Hz). MS (NH₃-CI): *m/e* 400 (7), 399 (37), 398 (26), 397 (100).

30 Example 524 spectral data: TLC R_f 0.50 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.89 (1H, s), 7.76 (1H, d, *J* = 9.1 Hz), 6.90-6.87 (2H, m), 4.35 (1H, v br), 3.86 (3H, s), 2.93 (2H, q, *J* = 7.6 Hz), 2.48 (3H, s), 2.39 (2H, br), 2.00-1.90 (2H, m), 1.43 (3H, t, *J* = 7.6 Hz), 1.38-1.22 (2H, m), 1.18-1.02 (2H, m), 0.90 (6H, t, *J* = 7.3 Hz). MS (NH₃-CI): *m/e* calc'd for C₂₂H₂₁N₄O: 367.2498, found 367.2506; 369 (3), 368 (25), 367 (100).

35 Example 526 spectral data: TLC R_f 0.28 (10:90 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.91 (1H, s), 7.69 (1H, d, *J* = 8.1 Hz), 7.34-7.30 (2H, m), 4.40-4.35 (1H, m), 2.93 (2H, q, *J* = 7.4 Hz), 2.44 (3H, s), 2.38 (2H, m), 1.96 (2H, m), 1.43 (3H, t, *J* =

7.5 Hz), 1.35-1.22 (2H, m), 1.15-1.05 (2H, m), 0.90 (6H, t, $J = 7.1$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 374 (8), 373 (35), 372 (25), 371 (100). Analysis calc'd for $\text{C}_{21}\text{H}_{27}\text{N}_4\text{Cl}$: C, 68.00; H, 7.35; N, 15.10; found: C, 67.89; H, 7.38; N, 14.94.

5 Example 528 spectral data: TLC R_f 0.65 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.97 (1H, s), 7.86 (1H, d, $J = 8.0$ Hz), 7.82 (1H, d, $J = 1.1$ Hz), 7.67 (1H, dd, $J = 8.0, 1.1$ Hz), 4.38 (1H, br), 2.95 (2H, q, $J = 7.5$ Hz), 2.39 (2H, br), 2.04-1.92 (2H, br), 1.42 (3H, t, $J = 7.5$ Hz), 1.40-1.21 (3H, m), 1.19-1.03 (1H, m), 0.91 (6H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 428 (8), 427 (37), 426 (27), 425 (100).

10 Example 538 spectral data: TLC R_f 0.56 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.96 (1H, s), 7.88 (1H, d, $J = 8.0$ Hz), 7.83 (1H, d, $J = 0.8$ Hz), 7.68 (1H, dd, $J = 8.0, 0.8$ Hz), 3.77 (1H, br), 2.95 (2H, q, $J = 7.5$ Hz), 2.61 (1H, br), 2.08 (1H, br), 1.45 (3H, t, $J = 7.5$ Hz), 1.36-1.25 (1H, m), 1.17 (3H, d, $J = 6.6$ Hz), 0.71 (3H, t, $J = 7.3$ Hz), 0.69 (3H, d, $J = 7.0$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 414 (7), 413 (33), 412 (24), 411 (100).

15 Example 534 spectral data: MS (ESI): m/e 363 ($M+2$), 361 (M^+ , 100 %).

Example 544 spectral data: TLC R_f 0.63 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.90 (1H, s), 7.74 (1H, d, $J = 9.1$ Hz), 6.89-6.86 (2H, m), 3.86 (3H, s), 3.79-3.73 (1H, m), 2.93 (3H, dq, $J = 7.7, 2.6$ Hz), 2.49 (3H, s), 2.03-1.99 (1H, m), 1.81 (3H, d, $J = 6.9$ Hz), 1.41 (3H, t, $J = 7.3$ Hz), 0.84-0.74 (2H, m), 0.53-0.41 (2H, m), 0.28-0.21 (1H, m).

20 Example 548 spectral data: TLC R_f 0.42 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.99 (1H, s), 7.84 (1H, d, $J = 7.7$ Hz), 7.82 (1H, d, $J = 0.9$ Hz), 7.68 (1H, dd, $J = 7.7, 0.9$ Hz), 3.83-3.70 (1H, m), 3.00-2.90 (2H, m), 2.09-1.98 (1H, m), 1.83 (3H, d, $J = 7.0$ Hz), 1.40 (3H, t, $J = 7.3$ Hz), 0.88-0.78 (1H, m), 0.57-0.41 (2H, m), 0.30-0.20 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e 398 (6), 397 (31), 396 (22), 395 (100).

25 Example 551 spectral data: TLC R_f 0.56 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.93 (1H, s), 6.94 (2H, s), 4.75 (1H, heptet, $J = 7.0$ Hz), 2.95 (2H, q, $J = 7.7$ Hz), 2.32 (3H, s), 2.04 (6H, s), 1.80 (6H, d, $J = 7.0$ Hz), 1.36 (3H, t, $J = 7.7$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 311 (4), 310 (34), 309 (100); Analysis calc'd for $\text{C}_{15}\text{H}_{24}\text{N}_4 \cdot 0.5\text{H}_2\text{O}$: C, 71.89; H, 7.94; N, 17.65; found: C, 71.59; H, 7.83; N, 17.41.

30 Example 558 spectral data: TLC R_f 0.53 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.98 (1H, s), 7.86-7.81 (2H, m), 7.67 (1H, dd, $J = 8.4, 1.1$ Hz), 4.60-4.48 (1H, m), 3.01-2.93 (2H, m), 2.49-2.35 (1H, m), 2.13-2.00 (1H, m), 1.76 (3H, d, $J = 7.0$ Hz), 1.41 (3H, t, $J = 7.5$ Hz), 1.40-1.20 (4H, m), 0.87 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 414 (8), 413 (38), 412 (27), 411 (100).

35 Example 564 spectral data: TLC R_f 0.34 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.89 (1H, s), 7.77 (1H, d, $J = 9.2$ Hz), 6.89 (2H, m), 4.30-4.20 (1H, m), 3.86 (3H, s), 2.93 (2H, q, $J = 7.5$ Hz), 2.48 (3H, s), 2.45-2.35 (2H, m), 2.10-1.95 (2H, m),

1.44 (3H, t, J = 7.5 Hz), 1.40-1.20 (3H, m), 1.10-0.95 (1H, m), 0.84 (3H, t, J = 7.3 Hz), 0.81 (3H, t, J = 7.3 Hz).

Example 571 spectral data: TLC R_f 0.40 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.89 (1H, s), 6.95 (2H, s), 4.51 (1H, br), 3.44-3.24 (4H, m), 2.96 (2H, q, J = 7.3 Hz), 2.95-2.87 (1H, m), 2.85-2.75 (1H, m), 2.59-2.49 (1H, m), 2.32 (3H, s), 2.27-2.18 (1H, m), 2.04 (3H, s), 2.04 (3H, s), 1.38 (3H, t, J = 7.7 Hz), 1.12 (3H, t, J = 7.0 Hz), 0.84 (3H, t, J = 7.3 Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{23}\text{H}_{33}\text{N}_4\text{O}$: 380.2576, found 380.2554; 383 (4), 382 (28), 381 (100).

Example 581 spectral data: TLC R_f 0.33 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.89 (1H, s), 6.95 (2H, s), 4.49-4.39 (1H, m), 4.23-4.13 (1H, m), 3.91 (1H, dd, J = 9.9, 4.8 Hz), 3.48 (1H, dq, J = 9.1, 7.0 Hz), 3.30 (1H, dq, J = 9.1, 7.0 Hz), 2.95 (2H, q, J = 7.7 Hz), 2.60-2.47 (1H, m), 2.32 (3H, s), 2.15-2.01 (1H, m), 2.04 (3H, s), 2.03 (3H, s), 1.37 (3H, t, J = 7.5 Hz), 1.00 (3H, t, J = 7.0 Hz), 0.86 (3H, t, J = 7.3 Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{23}\text{H}_{31}\text{N}_4\text{O}$: 367.2498, found 367.2497; 369 (4), 368 (27), 367 (100).

Example 591 spectral data: TLC R_f 0.42 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.91 (1H, s), 6.95 (2H, s), 3.76 (1H, br), 3.47-3.40 (1H, m), 3.21 (3H, s), 2.99-2.90 (1H, m), 2.88 (2H, q, J = 7.3 Hz), 2.76 (1H, br), 2.51-2.41 (1H, m), 2.32 (3H, s), 2.09 (1H, br), 2.08 (3H, s), 2.04 (3H, s), 1.35 (3H, t, J = 7.3 Hz), 0.84-0.76 (1H, m), 0.56-0.44 (2H, m), 0.30-0.21 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{23}\text{H}_{31}\text{N}_4\text{O}$: 379.2498, found 379.2514; 381 (4), 380 (27), 379 (100).

Example 690 spectral data: TLC R_f 0.12 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 9.01 (1H, s), 7.38-7.22 (5H, m), 6.75 (1H, s), 6.69 (1H, s), 5.48 (2H, s), 3.70 (3H, s), 2.84 (2H, q, J = 7.7 Hz), 2.37 (3H, s), 2.05 (3H, s), 1.26 (3H, t, J = 7.7 Hz). MS ($\text{NH}_3\text{-CI}$): m/e 375 (4), 374 (28), 373 (100).

Example 692 spectral data: TLC R_f 0.32 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.98 (1H, s), 7.48 (1H, s), 7.37-7.18 (5H, m), 7.11 (1H, s), 5.49 (2H, s), 2.84 (2H, q, J = 7.3 Hz), 2.38 (3H, s), 2.29 (6H, s), 1.31 (3H, t, J = 7.3 Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{23}\text{H}_{24}\text{N}_4$: 356.2001, found 356.1978; 359 (4), 358 (28), 357 (100).

Example 693 spectral data: TLC R_f 0.22 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.90 (1H, s), 7.78 (1H, d, J = 9.5 Hz), 6.90-6.87 (2H, m), 3.86 (3H, s), 3.62 (1H, br), 2.91 (2H, q, J = 7.5 Hz), 2.50 (3H, s), 2.40 (1H, br), 2.26-2.13 (1H, m), 1.92 (1H, br), 1.58 (1H, br), 1.43 (3H, t, J = 7.5 Hz), 1.35-1.25 (1H, m), 1.13-1.03 (1H, m), 0.95-0.75 (2H, m), 0.85 (3H, t, J = 7.1 Hz), 0.54-0.42 (2H, m), 0.22-0.17 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e 381 (4), 380 (25), 379 (100).

Example 697 spectral data: TLC R_f 0.28 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.89 (1H, s), 7.74 (1H, d, J = 9.5 Hz), 6.90-6.86 (2H, m), 4.58-4.45 (1H, m), 2.95 (2H, dq, J = 7.7, 2.2 Hz), 2.48 (3H, s), 2.45-2.35 (1H, m), 2.09-1.99 (1H, m),

1.74 (3H, d, $J = 7.0$ Hz), 1.42 (3H, t, $J = 7.5$ Hz), 1.37-1.23 (3H, m), 1.11-1.03 (1H, m), 0.86 (3H, t, $J = 7.0$ Hz).

Example 724 spectral data: TLC R_f 0.45 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.92 (1H, s), 7.75 (1H, d, $J = 8.4$ Hz), 7.09 (1H, d, $J = 2.6$ Hz), 6.96 (1H, dd, $J = 8.4, 2.6$ Hz), 3.87 (3H, s), 3.76 (1H, br), 2.94 (2H, q, $J = 7.3$ Hz), 2.61 (1H, br), 2.09 (1H, br), 1.45 (3H, t, $J = 7.3$ Hz), 1.36-1.26 (1H, m), 1.15 (3H, d, $J = 6.6$ Hz), 0.71 (3H, t, $J = 7.3$ Hz), 0.68 (3H, d, $J = 6.6$ Hz). MS (NH_3 -CI): m/e 377 (1), 376 (8), 375 (38), 374 (25), 373 (100).

Example 725 spectral data: TLC R_f 0.31 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.88 (1H, s), 7.80 (1H, d, $J = 9.2$ Hz), 6.89 (2H, m), 3.86 (3H, s), 3.75 (1H, m), 2.92 (2H, q, $J = 7.4$ Hz), 2.60 (1H, m), 2.48 (3H, s), 2.05 (1H, m), 1.46 (3H, t, $J = 7.4$ Hz), 1.16 (3H, d, $J = 7.0$ Hz), 0.70 (3H, t, $J = 7.3$ Hz), 0.67 (3H, d, $J = 6.6$ Hz).

Example 727 spectral data: TLC R_f 0.44 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.90 (1H, s), 7.84 (1H, d, $J = 2.2$ Hz), 7.74 (1H, d, $J = 8.4$ Hz), 7.65 (1H, dd, $J = 8.4, 2.2$ Hz), 3.76 (1H, br), 2.93 (1H, q, $J = 7.3$ Hz), 2.60 (1H, br), 2.08 (1H, br), 1.42 (3H, t, $J = 7.3$ Hz), 1.37-1.27 (1H, m), 1.16 (3H, d, $J = 7.0$ Hz), 0.69 (3H, t, $J = 7.3$ Hz), 0.67 (3H, d, $J = 7.0$ Hz). MS (NH_3 -CI): m/e 414 (7), 413 (33), 412 (27), 411 (100).

Example 750 spectral data: TLC R_f 0.42 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.94 (1H, s), 7.73 (1H, d, $J = 8.4$ Hz), 7.10 (1H, d, $J = 2.6$ Hz), 6.96 (1H, dd, $J = 8.4, 2.6$ Hz), 3.87 (3H, s), 3.63 (1H, v br), 2.92 (2H, q, $J = 7.3$ Hz), 2.38 (1H, br), 2.22-2.10 (1H, m), 1.94 (1H, br), 1.42 (3H, t, $J = 7.3$ Hz), 1.41-1.29 (1H, m), 1.23-1.08 (1H, m), 0.91 (3H, t, $J = 7.3$ Hz), 0.89-0.79 (1H, m), 0.51-0.41 (2H, m), 0.25-0.15 (1H, m). MS (NH_3 -CI): m/e 388 (8), 387 (34), 386 (25), 385 (100).

Example 751 spectral data: TLC R_f 0.36 (40:60 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.89 (1H, s), 7.77 (1H, d, $J = 9.1$ Hz), 6.90 (2H, m), 3.86 (3H, s), 3.62 (1H, m), 2.84 (2H, q, $J = 7.5$ Hz), 2.49 (3H, s), 2.40 (1H, m), 2.19 (1H, m), 1.90 (1H, m), 1.43 (3H, t, $J = 7.5$ Hz), 1.38 (1H, m), 1.19 (1H, m), 0.91 (3H, t, $J = 7.3$ Hz), 0.80 (1H, m), 0.49 (2H, m), 0.21 (1H, m).

Example 753 spectral data: TLC R_f 0.44 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.92 (1H, s), 7.84 (1H, d, $J = 1.8$ Hz), 7.73 (1H, d, $J = 8.5$ Hz), 7.65 (1H, dd, $J = 8.5, 1.8$ Hz), 3.65 (1H, br), 2.92 (1H, q, $J = 7.5$ Hz), 2.38 (1H, br), 2.25-2.14 (1H, m), 1.94 (1H, br), 1.43-1.26 (1H, m), 1.40 (3H, t, $J = 7.5$ Hz), 1.21-1.06 (1H, m), 0.92 (3H, t, $J = 7.3$ Hz), 0.91-0.79 (1H, m), 0.52-0.44 (2H, m), 0.22-0.16 (1H, m). MS (NH_3 -CI): m/e 426 (9), 425 (42), 424 (31), 423 (100).

Example 767 spectral data: MS (NH_3 -CI): m/e 379 ($\text{M}+\text{H}^+$, 100%).

Example 776 spectral data: TLC R_f 0.41 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.93 (1H, s), 7.73 (1H, d, $J = 8.4$ Hz), 7.09 (1H, d, $J = 2.6$ Hz), 6.96 (1H,

- dd, $J = 8.4, 2.6$ Hz), 4.28 (1H, br), 3.87 (3H, s), 2.95 (2H, q, $J = 7.3$ Hz), 2.41 (2H, br), 2.10-1.93 (2H, m), 1.43 (3H, t, $J = 7.3$ Hz), 1.40-1.23 (1H, m), 1.18-1.03 (1H, m), 0.91 (3H, t, $J = 7.3$ Hz), 0.82 (3H, t, $J = 7.5$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{30}\text{H}_{28}\text{ClN}_4\text{O}$: 373.1795, found 373.1815; 376 (8), 375 (35), 374 (24), 373 (100).
- 5 Example 777 spectral data: TLC R_f 0.46 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.89 (1H, s), 7.76 (1H, d, $J = 9.0$ Hz), 6.90-6.87 (2H, m), 4.29 (1H, br), 3.86 (3H, s), 2.94 (2H, q, $J = 7.4$ Hz), 2.48 (3H, s), 2.40 (2H, br), 2.10-1.92 (2H, m), 1.44 (3H, t, $J = 7.4$ Hz), 1.37-1.22 (1H, m), 1.18-1.02 (1H, m), 0.90 (3H, t, $J = 7.3$ Hz), 0.81 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{21}\text{H}_{29}\text{N}_4\text{O}$: 353.2341, found
- 10 353.2328; 355 (3), 354 (23), 353 (100).
- Example 778 spectral data: TLC R_f 0.58 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.97 (1H, s), 7.86 (1H, d, $J = 8.0$ Hz), 7.83 (1H, d, $J = 0.8$ Hz), 7.68 (1H, dd, $J = 8.0, 0.8$ Hz), 4.30 (1H, br), 2.96 (2H, q, $J = 7.5$ Hz), 2.41 (2H, br), 2.11-1.95 (2H, m), 1.43 (3H, t, $J = 7.5$ Hz), 1.42-1.22 (2H, m), 0.92 (3H, t, $J = 7.3$ Hz), 0.83
- 15 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 414 (8), 413 (39), 412 (28), 411 (100).
- Example 779 spectral data: TLC R_f 0.44 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.91 (1H, s), 7.84 (1H, d, $J = 1.8$ Hz), 7.72 (1H, d, $J = 8.0$ Hz), 7.65 (1H, dd, $J = 8.0, 1.8$ Hz), 4.31 (1H, br), 2.94 (1H, q, $J = 7.5$ Hz), 2.40 (2H, br), 2.10-1.93 (2H, m), 1.40 (3H, t, $J = 7.5$ Hz), 1.37-1.21 (1H, m), 1.19-1.02 (1H, m), 0.91 (3H, t, $J = 7.3$ Hz), 0.81 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 414 (9), 413 (43), 412 (31), 411
- 20 (100).
- Example 793 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 367 ($\text{M}+\text{H}^+$, 100%).
- Example 799 spectral data: TLC R_f 0.61 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.90 (1H, s), 7.47 (1H, s), 7.10 (1H, s), 4.28 (1H, br), 2.93 (2H, q, $J = 7.3$
- 25 Hz), 2.41 (1H, br), 2.36 (3H, s), 2.28 (6H, s), 2.07-1.91 (3H, m), 1.42 (3H, t, $J = 7.3$ Hz), 1.35-1.21 (1H, m), 1.19-1.03 (1H, m), 0.90 (3H, t, $J = 7.2$ Hz), 0.81 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{22}\text{H}_{30}\text{N}_4$: 350.2470, found 350.2476; 353 (3), 352 (24), 351 (100).
- Example 802 spectral data: TLC R_f 0.38 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.92 (1H, s), 7.84 (1H, d, $J = 1.8$ Hz), 7.73 (1H, d, $J = 8.4$ Hz), 7.65 (1H, dd, $J = 8.4, 1.8$ Hz), 3.53 (1H, br), 2.91 (1H, q, $J = 7.4$ Hz), 2.52-2.35 (1H, m), 2.34-2.20 (1H, m), 1.95 (1H, br), 1.40 (3H, t, $J = 7.4$ Hz), 0.89-0.79 (1H, m), 0.87 (3H, t, $J = 7.3$ Hz), 0.55-0.42 (2H, m), 0.25-0.15 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e 412 (8), 411 (41), 410 (29), 409 (100).
- 30
- 35 Example 803 spectral data: TLC R_f 0.33 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.93 (1H, s), 7.85 (1H, d, $J = 2.2$ Hz), 7.71 (1H, d, $J = 8.4$ Hz), 7.64 (1H, dd, $J = 8.4, 2.2$ Hz), 3.77 (1H, dq, $J = 9.9, 7.0$ Hz), 2.93 (1H, dq, $J = 7.5, 2.0$ Hz), 2.09-1.98 (1H, m), 1.82 (3H, d, $J = 7.0$ Hz), 1.39 (3H, t, $J = 7.5$ Hz), 0.86-0.78 (1H,

m), 0.59-0.50 (1H, m), 0.49-0.40 (1H, m), 0.29-0.20 (1H, m). MS (NH₃-CI): *m/e* 399 (2), 398 (8), 397 (39), 396 (24), 395 (100).

- Example 804 spectral data: TLC *R_f* 0.31 (20:80 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.92 (1H, s), 7.84 (1H, d, *J* = 1.8 Hz), 7.71-7.62 (2H, m), 4.55 (1H, m), 2.95 (2H, q, *J* = 7.5 Hz), 2.43-2.32 (1H, m), 2.10-1.98 (1H, m), 1.75 (3H, d, *J* = 7.0 Hz), 1.39 (3H, t, *J* = 7.5 Hz), 1.38-1.27 (1H, m), 1.19-1.09 (1H, m), 0.93 (3H, t, *J* = 7.1 Hz). MS (NH₃-CI): *m/e* 400 (7), 399 (32), 398 (22), 397 (100). Analysis calc'd for C₁₃H₂₀ClF₃N₄: C, 57.51; H, 5.08; N, 14.12; found: C, 57.55; H, 5.06; N, 13.95.
- Example 805 spectral data: TLC *R_f* 0.41 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.92 (1H, s), 7.84 (1H, d, *J* = 1.8 Hz), 7.70 (1H, d, *J* = 8.0 Hz), 7.64 (1H, dd, *J* = 8.0, 1.8 Hz), 4.58-4.49 (1H, m), 2.95 (1H, q, *J* = 7.5 Hz), 2.45-2.33 (1H, m), 2.11-2.00 (1H, m), 1.75 (3H, d, *J* = 6.6 Hz), 1.39 (3H, t, *J* = 7.5 Hz), 1.38-1.21 (4H, m), 0.86 (3H, t, *J* = 7.0 Hz). MS (NH₃-CI): *m/e* 414 (8), 413 (40), 412 (29), 411 (100).
- Example 807 spectral data: TLC *R_f* 0.49 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.91 (1H, s), 7.84 (1H, d, *J* = 1.8 Hz), 7.73 (1H, d, *J* = 8.4 Hz), 7.65 (1H, dd, *J* = 8.4, 1.8 Hz), 4.38-4.19 (1H, m), 2.94 (1H, q, *J* = 7.5 Hz), 2.40 (2H, br), 2.10-1.98 (2H, m), 1.41 (3H, t, *J* = 7.5 Hz), 1.38-1.20 (3H, m), 1.09-0.99 (1H, m), 0.84 (3H, t, *J* = 7.0 Hz), 0.81 (3H, t, *J* = 7.5 Hz). MS (NH₃-CI): *m/e* 428 (7), 427 (32), 426 (25), 425 (100).
- Example 808 spectral data: TLC *R_f* 0.51 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.91 (1H, s), 7.84 (1H, d, *J* = 1.8 Hz), 7.72 (1H, d, *J* = 8.4 Hz), 7.64 (1H, dd, *J* = 8.4, 1.8 Hz), 4.37 (1H, br), 2.93 (1H, q, *J* = 7.5 Hz), 2.38 (2H, br), 2.02-1.90 (2H, m), 1.40 (3H, t, *J* = 7.5 Hz), 1.38-1.20 (2H, m), 1.18-1.01 (2H, m), 0.90 (6H, t, *J* = 7.3 Hz). MS (NH₃-CI): *m/e* 428 (8), 427 (39), 426 (30), 425 (100).
- Example 809 spectral data: TLC *R_f* 0.40 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.90 (1H, s), 7.84 (1H, d, *J* = 2.2 Hz), 7.72 (1H, d, *J* = 8.1 Hz), 7.65 (1H, dd, *J* = 8.1, 2.2 Hz), 4.20 (1H, br), 2.94 (1H, q, *J* = 7.5 Hz), 2.51-2.38 (2H, m), 2.13-2.00 (2H, m), 1.41 (3H, t, *J* = 7.5 Hz), 0.82 (6H, t, *J* = 7.5 Hz). MS (NH₃-CI): *m/e* 400 (7), 399 (36), 398 (25), 397 (100).
- Example 824 spectral data: TLC *R_f* 0.27 (20:80 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.94 (1H, s), 8.10 (1H, s), 7.94 (1H, d, *J* = 8.8 Hz), 7.87 (1H, d, *J* = 8.1 Hz), 4.56 (1H, m), 2.96 (2H, q, *J* = 7.5 Hz), 2.40 (1H, m), 2.10-2.00 (1H, m), 1.76 (3H, d, *J* = 7.0 Hz), 1.39 (3H, t, *J* = 7.5 Hz), 1.33-1.10 (2H, m), 0.93 (3H, t, *J* = 7.1 Hz). ¹⁹F NMR (300 MHz, CDCl₃): δ -58.2, -63.4. MS (NH₃-CI): *m/e* 433 (3), 432 (24), 431 (100).
- Example 832 spectral data: TLC *R_f* 0.34 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.94 (1H, s), 7.73 (1H, d, *J* = 8.5 Hz), 7.10 (1H, d, *J* = 2.6 Hz), 6.96 (1H, dd, *J* = 8.5, 2.6 Hz), 3.87 (3H, s), 3.55 (1H, br), 2.92 (2H, q, *J* = 7.3 Hz), 2.53-2.35 (1H, m), 2.31-2.18 (1H, m), 1.96 (1H, br), 1.42 (3H, t, *J* = 7.3 Hz), 0.87 (3H, t, *J* =

7.5 Hz), 0.87-0.79 (1H, m), 0.53-0.43 (2H, m), 0.25-0.15 (1H, m). MS (NH_3 -CI): m/e 374 (8), 373 (34), 372 (24), 371 (100).

Example 833 spectral data: TLC R_f 0.20 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.96 (1H, s), 7.70 (1H, d, $J = 8.4$ Hz), 7.10 (1H, d, $J = 2.5$ Hz), 6.96 (1H, dd, $J = 8.4, 2.5$ Hz), 4.16 (2H, d, $J = 7.0$ Hz), 3.87 (3H, s), 3.01 (2H, q, $J = 7.3$ Hz), 1.46 (3H, t, $J = 7.3$ Hz), 1.37-1.27 (1H, m), 0.66-0.52 (4H, m). MS (NH_3 -CI): m/e 346 (6), 345 (32), 344 (23), 343 (100).

Example 834 spectral data: TLC R_f 0.18 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.94 (1H, s), 7.69 (1H, d, $J = 8.4$ Hz), 7.09 (1H, d, $J = 1$ Hz), 6.96 (1H, dd, $J = 8.4, 1$ Hz), 4.60-4.50 (1H, m), 3.87 (3H, s), 2.97 (2H, q, $J = 7.3$ Hz), 2.49-2.33 (1H, m), 2.09-1.97 (1H, m), 1.74 (3H, d, $J = 7.0$ Hz), 1.41 (3H, t, $J = 7.5$ Hz), 1.40-1.22 (1H, m), 1.21-1.09 (1H, m), 0.92 (3H, t, $J = 7.1$ Hz). MS (NH_3 -CI): m/e calc'd for $\text{C}_{19}\text{H}_{21}\text{ClN}_2\text{O}$: 359.1639, found 359.1623; 362 (7), 361 (33), 360 (23), 359 (100). Analysis calc'd for $\text{C}_{19}\text{H}_{21}\text{ClN}_2\text{O} \cdot 0.5 \text{H}_2\text{O}$: C, 62.20; H, 6.32; N, 15.27; found: C, 62.33; H, 6.36; N, 14.86.

Example 835 spectral data: TLC R_f 0.39 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.94 (1H, s), 7.69 (1H, d, $J = 8.4$ Hz), 7.09 (1H, d, $J = 2.5$ Hz), 6.95 (1H, dd, $J = 8.4, 2.5$ Hz), 4.53-4.47 (1H, m), 3.87 (3H, s), 3.01-2.92 (2H, m), 2.48-2.35 (1H, m), 2.11-1.99 (1H, m), 1.74 (3H, d, $J = 6.9$ Hz), 1.41 (3H, t, $J = 7.5$ Hz), 1.38-1.22 (3H, m), 1.14-1.00 (1H, m), 0.86 (3H, t, $J = 7.1$ Hz). MS (NH_3 -CI): m/e 376 (7), 375 (33), 374 (23), 373 (100).

Example 836 spectral data: TLC R_f 0.42 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.94 (1H, s), 7.79 (1H, d, $J = 8.8$ Hz), 7.09 (1H, d, $J = 2.5$ Hz), 6.95 (1H, dd, $J = 8.8, 2.5$ Hz), 4.55-4.47 (1H, m), 3.87 (3H, s), 3.01-2.92 (2H, m), 2.48-2.35 (1H, m), 2.10-1.97 (1H, m), 1.74 (3H, d, $J = 7.0$ Hz), 1.41 (3H, t, $J = 7.5$ Hz), 1.35-1.20 (5H, m), 1.18-1.02 (1H, m), 0.84 (3H, t, $J = 7.0$ Hz). MS (NH_3 -CI): m/e calc'd for $\text{C}_{21}\text{H}_{23}\text{ClN}_2\text{O}$: 387.1952, found 387.1944; 391 (1), 390 (8), 389 (35), 388 (25), 387 (100).

Example 837 spectral data: TLC R_f 0.45 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.93 (1H, s), 7.73 (1H, d, $J = 8.8$ Hz), 7.09 (1H, d, $J = 2.6$ Hz), 6.96 (1H, dd, $J = 8.8, 2.6$ Hz), 4.25 (1H, br), 3.87 (3H, s), 2.95 (2H, q, $J = 7.3$ Hz), 2.41 (2H, br), 2.10-2.00 (2H, m), 1.43 (3H, t, $J = 7.3$ Hz), 1.37-1.20 (3H, m), 1.12-0.98 (1H, m), 0.84 (3H, t, $J = 7.3$ Hz), 0.82 (3H, t, $J = 7.4$ Hz). MS (NH_3 -CI): m/e 390 (8), 389 (34), 388 (25), 387 (100).

Example 838 spectral data: TLC R_f 0.48 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.94 (1H, s), 7.72 (1H, d, $J = 8.5$ Hz), 7.09 (1H, d, $J = 2.2$ Hz), 6.96 (1H, dd, $J = 8.5, 2.2$ Hz), 4.36 (1H, v br), 3.87 (3H, s), 2.94 (2H, q, $J = 7.3$ Hz), 2.39 (2H, br), 2.02-1.90 (2H, m), 1.42 (3H, t, $J = 7.3$ Hz), 1.39-1.21 (2H, m), 1.18-1.03 (2H, m), 0.90 (6H, t, $J = 7.3$ Hz). MS (NH_3 -CI): m/e calc'd for $\text{C}_{21}\text{H}_{23}\text{ClN}_2\text{O}$: 387.1952, found 387.1958; 391 (1), 390 (8), 389 (34), 388 (26), 387 (100).

Example 839 spectral data: TLC R_f 0.36 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.93 (1H, s), 7.73 (1H, d, $J = 8.5$ Hz), 7.09 (1H, d, $J = 2.6$ Hz), 6.96 (1H, dd, $J = 8.5, 2.6$ Hz), 4.19 (1H, br s), 3.87 (3H, s), 2.96 (2H, q, $J = 7.5$ Hz), 2.52-2.38 (2H, m), 2.13-1.99 (2H, m), 1.43 (3H, t, $J = 7.5$ Hz), 0.83 (6H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{11}\text{H}_{14}\text{ClN}_4\text{O}$: 359.1639, found 359.1632; 362 (7), 361 (34), 360 (23), 359 (100).

Example 870 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 423 ($\text{M}+\text{H}^+$, 100%).

Example 900 spectral data: TLC R_f 0.38 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.93 (1H, s), 7.75 (1H, d, $J = 9.2$ Hz), 6.90-6.86 (2H, m), 4.23 (2H, t, $J = 7.7$ Hz), 3.86 (3H, s), 2.95 (2H, q, $J = 7.7$ Hz), 2.48 (3H, s), 1.93-1.83 (2H, m), 1.45 (3H, t, $J = 7.6$ Hz), 1.43-1.36 (4H, m), 0.92 (3H, t, $J = 7.0$ Hz).

Example 902 spectral data: TLC R_f 0.28 (5:95 ethyl acetate-dichloromethane). ^1H NMR (300 MHz, CDCl_3): δ 8.94 (1H, s), 7.63 (1H, d, $J = 8.1$ Hz), 7.37 (1H, d, $J = 1.0$ Hz), 7.21 (1H, dd, $J = 8.1, 1.0$ Hz), 4.38 (1H, br), 2.94 (2H, q, $J = 7.5$ Hz), 2.41 (3H, s), 2.40 (2H, br), 2.00-1.90 (2H, m), 1.42 (3H, t, $J = 7.5$ Hz), 1.35-1.22 (2H, m), 1.17-1.03 (2H, m), 0.90 (6H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{21}\text{H}_{28}\text{ClN}_4$: 371.2002, found 371.1993; 374 (8), 373 (34), 372 (25), 371 (100).

Example 944 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 377 ($\text{M}+\text{H}^+$, 100%).

Example 945 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 365 ($\text{M}+\text{H}^+$, 100%).

Example 947 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 353 ($\text{M}+\text{H}^+$, 100%).

Example 951 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 381 ($\text{M}+\text{H}^+$, 100%).

Example 952 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 353 ($\text{M}+\text{H}^+$, 100%).

Example 1003 spectral data: TLC R_f 0.10 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.99 (1H, s), 7.43 (1H, s), 7.19 (2H, d, $J = 8.8$ Hz), 6.86 (2H, d, $J = 8.8$ Hz), 6.84 (1H, s), 5.42 (2H, s), 3.94 (3H, s), 3.91 (3H, s), 3.78 (3H, s), 2.86 (2H, q, $J = 7.7$ Hz), 2.45 (3H, s), 1.35 (3H, t, $J = 7.7$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 421 (4), 420 (27), 419 (100). Analysis calculated for $\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_3$: C, 68.88; H, 6.26; N, 13.39; found: C, 68.53; H, 6.30; N, 12.96.

Example 1012 spectral data: m.p. 147-148 °C. TLC R_f 0.18 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.88 (1H, s), 7.60 (1H, s), 6.77 (1H, s), 4.61 (2H, t, $J = 8.6$ Hz), 3.44 (1H, v br), 3.24 (2H, t, $J = 8.6$ Hz), 2.94 (2H, br), 2.44 (3H, s), 2.03 (2H, v br), 1.45 (3H, br t, $J = 6$ Hz), 0.89-0.79 (2H, m), 0.58 (2H, br), 0.50-0.40 (2H, m), 0.27-0.17 (2H, m). MS ($\text{NH}_3\text{-CI}$): m/e 377 (4), 376 (27), 375 (100). Analysis calc'd for $\text{C}_{22}\text{H}_{26}\text{N}_4\text{O}$: C, 73.77; H, 7.01; N, 14.96; found: C, 73.69; H, 7.08; N, 14.40.

Example 1023 spectral data: TLC R_f 0.22 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 9.04 (1H, s), 7.78 (1H, d, $J = 8.4$ Hz), 7.44 (1H, d, $J = 1.1$ Hz), 7.30 (1H, dd, $J = 8.4, 1.1$ Hz), 7.20 (2H, d, $J = 8.5$ Hz), 6.87 (2H, d, $J = 8.5$ Hz), 5.44 (2H, s), 3.79 (3H, s), 2.90 (2H, q, $J = 7.5$ Hz), 1.32 (3H, t, $J = 7.5$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 467 (1), 466 (8), 465 (35), 464 (27), 463 (100).

- Example 1027 spectral data: TLC R_f 0.41 (25:75 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.96 (1H, s), 7.76 (1H, d, $J = 8.4$ Hz), 7.45-7.44 (1H, m), 7.27 (1H, dm, $J = 8$ Hz), 4.61-4.51 (1H, m), 2.98 (2H, dq, $J = 7.5, 1.6$ Hz), 2.48-2.35 (1H, m), 2.10-1.98 (1H, m), 1.75 (3H, d, $J = 7.0$ Hz), 1.41 (3H, t, $J = 7.5$ Hz), 1.35-1.22 (2H, m), 0.93 (3H, t, $J = 7.2$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{11}\text{H}_{21}\text{ClF}_3\text{N}_4\text{O}$: 413.1349, found 413.1344; 416 (8), 415 (35), 414 (24), 413 (100).
- Example 1028 spectral data: TLC R_f 0.45 (25:75 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.96 (1H, s), 7.77 (1H, d, $J = 8.4$ Hz), 7.44 (1H, m), 7.27 (1H, dm, $J = 8$ Hz), 4.57-4.49 (1H, m), 2.97 (2H, dq, $J = 7.7, 1.7$ Hz), 2.47-2.36 (1H, m), 2.12-2.02 (1H, m), 1.75 (3H, d, $J = 7.0$ Hz), 1.41 (3H, t, $J = 7.7$ Hz), 1.33-1.21 (4H, m), 0.86 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{20}\text{H}_{23}\text{ClF}_3\text{N}_4\text{O}$: 427.1509, found 427.1507; 430 (8), 429 (35), 428 (25), 427 (100).
- Example 1032 spectral data: TLC R_f 0.44 (25:75 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.95 (1H, s), 7.80 (1H, d, $J = 8.4$ Hz), 7.45-7.44 (1H, m), 7.30 (1H, dm, $J = 8$ Hz), 4.23-4.17 (1H, m), 2.97 (2H, q, $J = 7.6$ Hz), 2.54-2.39 (2H, m), 2.14-2.00 (2H, m), 1.43 (3H, t, $J = 7.6$ Hz), 0.84 (6H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{19}\text{H}_{21}\text{ClF}_3\text{N}_4\text{O}$: 413.1368, found 413.1373; 416 (8), 415 (34), 414 (24), 413 (100).
- Example 1150 spectral data: TLC R_f 0.23 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.90 (1H, s), 7.73 (1H, d, $J = 8.8$ Hz), 7.36 (1H, d, $J = 2.6$ Hz), 7.17 (1H, dd, $J = 8.8, 2.6$ Hz), 3.92 (3H, s), 3.70-3.55 (1H, m), 2.91 (2H, q, $J = 7.4$ Hz), 2.45-2.35 (1H, m), 2.25-2.15 (1H, m), 2.00-1.90 (1H, m), 1.40 (3H, t, $J = 7.4$ Hz), 1.40-1.30 (1H, m), 1.20-1.10 (1H, m), 0.91 (3H, t, $J = 7.2$ Hz), 0.87-0.77 (1H, m), 0.54-0.44 (2H, m), 0.25-0.15 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{22}\text{H}_{24}\text{F}_3\text{N}_4\text{O}$: 419.2057, found 419.2058; 421 (3), 420 (25), 419 (100).
- Example 1153 spectral data: TLC R_f 0.48 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 9.00 (1H, s), 7.89 (1H, d, $J = 8.0$ Hz), 7.84 (1H, s), 7.69 (1H, d, $J = 8.0$ Hz), 7.40-7.30 (5H, m), 5.14 (1H, d, $J = 10.2$ Hz), 2.82 (1H, dq, $J = 15.5, 7.7$ Hz), 2.68 (1H, dq, $J = 15.5, 7.7$ Hz), 2.15 (1H, br), 1.23 (3H, t, $J = 7.7$ Hz), 1.13-1.03 (1H, m), 0.78-0.62 (2H, m), 0.53-0.43 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{24}\text{H}_{21}\text{ClF}_3\text{N}_4$: 457.1407, found 457.1389; 460 (9), 459 (35), 458 (29), 457 (100).
- Example 1155 spectral data: TLC R_f 0.46 (25:75 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.98 (1H, s), 7.83 (1H, d, $J = 8.4$ Hz), 7.46-7.27 (7H, m), 5.13 (1H, d, $J = 10.7$ Hz), 2.88-2.62 (2H, m), 2.15 (1H, br), 1.26 (3H, t, $J = 7.5$ Hz), 1.12-1.02 (1H, m), 0.78-0.62 (2H, m), 0.54-0.44 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{22}\text{H}_{21}\text{ClF}_3\text{N}_4\text{O}$: 473.1361, found 473.1365; 476 (9), 475 (36), 474 (29), 473 (100).
- Example 1157 spectral data: TLC R_f 0.19 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.93 (1H, s), 7.77 (1H, d, $J = 8.8$ Hz), 7.40-7.30 (6H, m), 7.19 (1H, dd, $J = 8.8, 2.2$ Hz), 5.13 (1H, d, $J = 10.6$ Hz), 3.92 (3H, s), 2.79 (1H, dq, $J = 15, 7.7$ Hz), 2.64 (1H, dq, $J = 15, 7.7$ Hz), 2.12 (1H, br), 1.21 (3H, t, $J = 7.7$ Hz), 1.10-1.00 (1H,

m), 0.77-0.62 (2H, m), 0.55-0.45 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{23}\text{H}_{24}\text{F}_3\text{N}_4\text{O}$: 453.1902, found 453.1903; 455 (4), 454 (28), 453 (100).

Example 1158 spectral data: TLC R_f 0.16 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.98 (1H, s), 7.46-7.25 (7H, m), 5.12 (1H, br d, $J = 9$ Hz), 2.85-2.62 (2H, m), 2.14 (1H, br), 2.13 (3H, d, $J = 0.7$ Hz), 1.18 (3H, dq, $J = 7.7, 4.1$ Hz), 0.75-0.35 (4H, m). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{24}\text{H}_{23}\text{Cl}_2\text{N}_4$: 437.1300, found 437.1294; 440 (19), 439 (67), 438 (32), 437 (100).

Example 1161 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 441 ($\text{M}+\text{H}^+$, 100%).

Example 1163 spectral data: TLC R_f 0.44 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 9.00 (1H, s), 7.89 (1H, d, $J = 8.4$ Hz), 7.84 (1H, s), 7.69 (1H, d, $J = 8.4$ Hz), 7.38 (2H, d, $J = 9$ Hz), 7.05 (2H, d, $J = 9$ Hz), 5.08 (1H, d, $J = 10.2$ Hz), 2.82 (1H, dq, $J = 15.5, 7.7$ Hz), 2.68 (1H, dq, $J = 15.5, 7.7$ Hz), 2.14 (1H, m), 1.25 (3H, t, $J = 7.7$ Hz), 1.10-1.01 (1H, m), 0.74-0.62 (2H, m), 0.51-0.41 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{24}\text{H}_{20}\text{ClF}_4\text{N}_4$: 475.1313, found 475.1307; 479 (1), 478 (9), 477 (35), 476 (30), 475 (100).

Example 1222 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 363 ($\text{M}+\text{H}^+$, 100%).

Example 1252 spectral data: TLC R_f 0.24 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.72 (1H, s), 7.87 (1H, dd, $J = 8.8, 5.5$ Hz), 7.46 (1H, dd, $J = 8.8, 2.5$ Hz), 7.35-7.26 (1H, m), 7.24-7.18 (6H, m), 7.08-7.01 (4H, m), 4.89-4.79 (1H, m), 4.49 (2H, d, $J = 12.1$ Hz), 4.37 (2H, d, $J = 12.1$ Hz), 4.27 (2H, t, $J = 9.3$ Hz), 4.01 (2H, dd, $J = 9.9, 5.2$ Hz), 2.98 (2H, q, $J = 7.7$ Hz), 1.39 (3H, t, $J = 7.7$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{21}\text{H}_{25}\text{F}_4\text{N}_4\text{O}_2$: 565.2227, found 565.2226; 567 (7), 566 (36), 565 (100).

Example 1255 spectral data: TLC R_f 0.50 (25:75 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.96 (1H, s), 7.80 (1H, d, $J = 8.4$ Hz), 7.45-7.43 (1H, m), 7.31-7.27 (1H, dm, $J = 8$ Hz), 3.80-3.73 (1H, m), 2.93 (2H, q, $J = 7.3$ Hz), 2.40 (1H, br), 2.25-2.14 (1H, m), 1.95 (1H, br), 1.42 (3H, t, $J = 7.5$ Hz), 1.35-1.10 (2H, m), 0.92 (3H, t, $J = 7.3$ Hz), 0.91-0.80 (1H, m), 0.53-0.44 (2H, m), 0.24-0.14 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{21}\text{H}_{23}\text{ClF}_4\text{N}_4\text{O}$: 439.1519, found 439.1524; 442 (8), 441 (34), 440 (26), 439 (100).

Example 1256 spectral data: TLC R_f 0.48 (25:75 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.95 (1H, s), 7.79 (1H, d, $J = 8.4$ Hz), 7.45-7.43 (1H, m), 7.27 (1H, dm, $J = 8$ Hz), 4.35-4.25 (1H, m), 2.96 (2H, q, $J = 7.4$ Hz), 2.42 (2H, br), 2.12-1.93 (2H, m), 1.43 (3H, t, $J = 7.4$ Hz), 1.37-1.22 (2H, m), 0.91 (3H, t, $J = 7.2$ Hz), 0.83 (3H, t, $J = 7.5$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{20}\text{H}_{21}\text{ClF}_4\text{N}_4\text{O}$: 427.1514, found 427.1515; 430 (8), 429 (34), 428 (25), 427 (100).

Example 1295 spectral data: TLC R_f 0.37 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.91 (1H, s), 7.38 (1H, s), 6.83 (1H, s), 4.46 (1H, m, $J = 7.3$ Hz), 3.94 (3H, s), 3.91 (3H, s), 2.96 (2H, q, $J = 7.6$ Hz), 2.49-2.39 (1H, m), 2.43 (3H, s), 2.12-2.02 (1H, m), 1.75 (3H, d, $J = 6.5$ Hz), 1.44 (3H, t, $J = 7.5$ Hz), 0.86 (3H, t, $J = 7.5$ Hz).

MS (NH₃-CI): m/e calc'd for C₂₀H₂₁N₄O₂: 355.2134, found 355.2139; 357 (3), 356 (23), 355 (100).

Example 1296 spectral data: TLC R_f 0.37 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.00 (1H, s), 7.68 (1H, d, J = 8.4 Hz), 7.57 (1H, d, J = 2.2 Hz), 7.39 (1H, dd, J = 8.4, 2.2 Hz), 7.27 (2H, d, J = 8.4 Hz), 6.89 (2H, d, J = 8.4 Hz), 5.56 (1H, dd, J = 9.7, 7.4 Hz), 3.79 (3H, s), 2.92-2.75 (3H, m), 2.65-2.55 (1H, m), 1.31 (3H, t, J = 7.5 Hz), 0.92 (3H, t, J = 6.6 Hz). MS (NH₃-CI): m/e calc'd for C₂₃H₂₃Cl₂N₄O: 441.1249, found 441.1247; 445 (12), 444 (18), 443 (67), 442 (30), 441 (100).

Example 1319 spectral data: MS (NH₃-CI): m/e 459 (M+H⁺, 100%).

10 Example 1320 spectral data: ¹H NMR (300 MHz, CDCl₃): δ 8.99 (s, 1H), 7.68 (d, 1H, J = 8.4 Hz), 7.58 (d, 1H, J = 1.9 Hz), 7.42-7.3 (m, 6H), 6.04 (q, 1H), 2.82, (m, 2H), 2.16 (d, 3H, J = 7.4 Hz), 1.27 (t, 3H, J = 7.3, 7.7 Hz).

Example 1321 7906-5 spectral data: ¹H NMR (300 MHz, CDCl₃): δ 9.02 (s, 1H), 7.98 (d, 1H), 7.71 (d, 1H), 7.57 (d, 1H), 7.42-7.26 (m, 3H), 7.15 (m, 1H), 5.38 (d, 1H), 2.65 (m, 1H), 2.4 (m, 1H), 1.85 (m, 1H), 1.82 (s, 3H), 0.97 (t, 3H), 0.8 (m, 2H), 0.6 (m, 2H).

Example 1322 spectral data: MS (NH₃-CI): m/e 437 (M+H⁺, 100%).

Example 1323 spectral data: MS (NH₃-CI): m/e 455 (M+H⁺, 100%).

Example 1324 spectral data: MS (ESI): m/e 425 (M+H⁺), 381 (M +H⁺ -CO₂, 100%).

20 Example 1325 spectral data: MS (NH₃-CI): m/e 413 (M+H⁺, 100%).

Example 1326 spectral data: MS (NH₃-CI): m/e 427 (M+H⁺, 100%).

Example 1327 spectral data: MS (NH₃-CI): m/e 427 (M+H⁺, 100%).

Example 1328 spectral data: MS (NH₃-CI): m/e 427 (M+H⁺, 100%).

Example 1329 spectral data: MS (NH₃-CI): m/e 423 (M+H⁺, 100%).

25 Example 1330 spectral data: MS (NH₃-CI): m/e 418 (M+H⁺, 100%).

Example 1331 spectral data: MS (NH₃-CI): m/e 418 (M+H⁺, 100%).

Example 1332 spectral data: MS (NH₃-CI): m/e 499 (M+H⁺, 100%).

Example 1333 spectral data: MS (NH₃-CI): m/e 453 (M+H⁺, 100%).

Example 1334 spectral data: MS (NH₃-CI): m/e 423 (M+H⁺, 100%).

30 Example 1335 spectral data: MS (NH₃-CI): m/e 372 (M+H⁺, 100%).

Example 1337 spectral data: MS (NH₃-CI): m/e 443 (M+H⁺, 100%).

Example 1338 spectral data: MS (NH₃-CI): m/e 427 (M+H⁺, 100%).

Example 1339 spectral data: MS (NH₃-CI): m/e 379 (M+H⁺, 100%).

Example 1341 spectral data: MS (NH₃-CI): m/e 393 (M+H⁺, 100%).

35 Example 1342 spectral data: MS (NH₃-CI): m/e 378 (M+H⁺, 100%).

Example 1343 spectral data: MS (NH₃-CI): m/e 346 (M+H⁺, 100%).

Example 1344 spectral data: MS (NH₃-CI): m/e 363 (M+H⁺, 100%).

Example 1346 spectral data: MS (NH₃-CI): m/e 416 (M+H⁺, 100%).

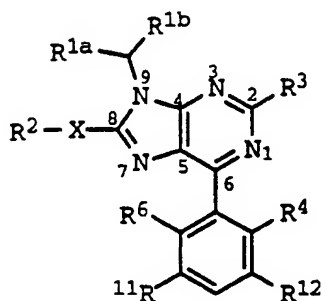
Example 1370 spectral data: TLC R_f 0.23 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.89 (1H, s), 7.72 (1H, d, J = 8.4 Hz), 7.35 (1H, d, J = 2.5 Hz), 7.17 (1H, dd, J = 8.4, 2.5 Hz), 4.27 (1H, br), 3.91 (3H, s), 2.93 (2H, q, J = 7.7 Hz), 2.40 (2H, br), 2.10-1.95 (2H, m), 1.41 (3H, t, J = 7.7 Hz), 1.39-1.27 (1H, m), 1.20-1.07 (1H, m), 0.91 (3H, t, J = 7.3 Hz), 0.81 (3H, t, J = 7.5 Hz). MS (NH_3 -CI): m/e calc'd for $\text{C}_{22}\text{H}_{26}\text{F}_2\text{N}_4\text{O}$: 407.2058, found 407.2052; 409 (3), 408 (24), 407 (100).

Example 1371 spectral data: MS (ESI): m/e 377 ($M+2$), 375 (M^+ , 100 %).

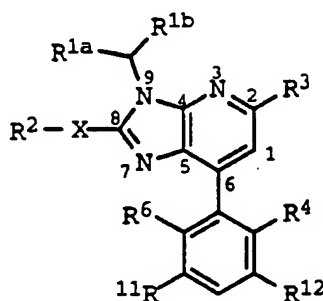
(b) Q1 = 2-tetrazolyl

(c) Q2 = 1,2,4-triazol-2-yl

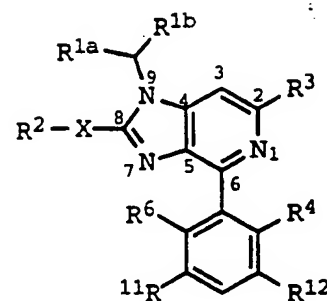
TABLE 1A



(A)



(B)



(C)

| Ex. No. | R ² | X | R ³ | R ⁴ | R ¹² | R ¹¹ | R ⁶ | R ^{1a} | R ^{1b} | mp, °C |
|---------|-----------------|-----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|-------------------------------|--------|
| 1043 | CH ₃ | CH ₂ | H | CH ₃ | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | oil |

20 Key:

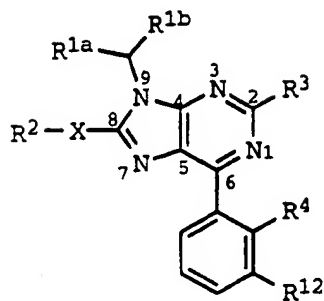
(a) Where the compound is indicated as an "oil", data is provided below:

Example 1043 spectral data: TLC R_f 0.40 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.91 (1H, s), 7.43 (1H, s), 7.10 (1H, s), 4.60-4.50 (1H, m), 2.94 (2H, dq, J = 7.5, 2.0 Hz), 2.45-2.35 (1H, m), 2.35 (3H, s), 2.28 (6H, s), 2.07-1.97 (1H, m), 1.73 (3H, d, J = 6.9 Hz), 1.41 (3H, t, J = 7.5 Hz), 1.40-1.27 (1H, m), 1.20-1.07 (1H, m), 0.92 (3H, t, J = 7.3 Hz). MS (NH_3 -CI): m/e calc'd for $\text{C}_{21}\text{H}_{29}\text{N}_4$: 337.2392, found

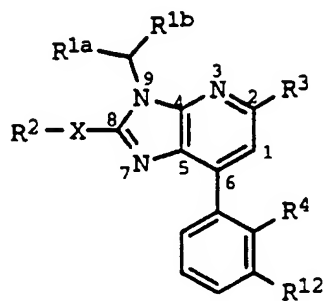
337.2396; 339 (3), 338 (23), 337 (100). Analysis calc'd for $C_{21}H_{29}N_4$: C, 74.96; H, 8.40; N, 16.65; found: C, 74.28; H, 8.02; N, 16.37.

5

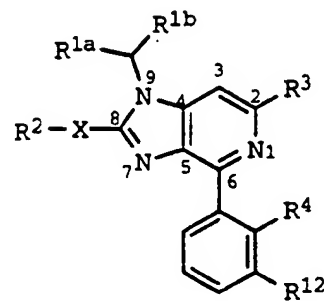
TABLE 1B



(A)



(B)



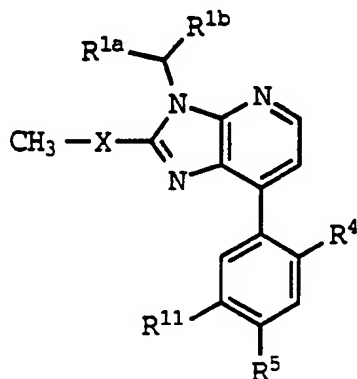
(C)

10

| Ex. No. | R ² | X | R ⁴ | R ⁵ | R ^{1a} | R ^{1b} | mp, °C |
|---------|-----------------|-----------------|---|---|---------------------------------|---------------------------------|--------|
| 1270 | CH ₃ | CH ₂ | CF ₃ | O(CH ₂) ₂ -OH | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1271 | CH ₃ | CH ₂ | CF ₃ | OCH ₂ CO ₂ -C ₂ H ₅ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1272 | CH ₃ | CH ₂ | CF ₃ | OCH ₂ CO-N(CH ₃) ₂ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1273 | CH ₃ | CH ₂ | CF ₃ | O(CH ₂) ₂ -NMe ₃ ⁺ Cl ⁻ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1274 | CH ₃ | CH ₂ | CF ₃ | OCH ₂ CH-(OH)C ₂ H ₅ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 1275 | CH ₃ | CH ₂ | OCH ₂ OCH ₃ | CH ₃ | CH ₃ | C ₃ H ₇ | 77-79 |
| 1276 | CH ₃ | CH ₂ | OH | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 1277 | CH ₃ | CH ₂ | OC ₂ H ₅ | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 1278 | CH ₃ | CH ₂ | OC ₃ H ₇ | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 1279 | CH ₃ | CH ₂ | O(CH ₂) ₂ -OH | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 1280 | CH ₃ | CH ₂ | OCH ₂ CO ₂ -C ₂ H ₅ | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 1281 | CH ₃ | CH ₂ | OCH ₂ CO-N(CH ₃) ₂ | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 1282 | CH ₃ | CH ₂ | O(CH ₂) ₂ -NMe ₃ ⁺ Cl ⁻ | CH ₃ | CH ₃ | C ₃ H ₇ | - |

| | | | | | | | |
|------|-----------------|-----------------|---|-----------------|-----------------|-------------------------------|---|
| 1283 | CH ₃ | CH ₂ | OCH ₂ CH- (OH)C ₂ H ₅ | CH ₃ | CH ₃ | C ₃ H ₇ | - |
|------|-----------------|-----------------|---|-----------------|-----------------|-------------------------------|---|

5 **TABLE 1C**



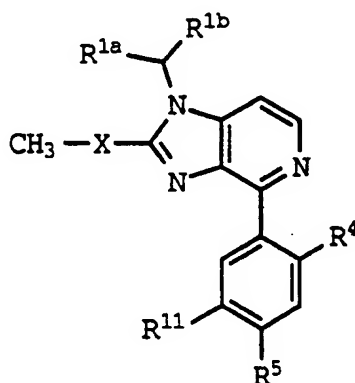
| Ex. No. | X | R ⁴ | R ⁵ | R ¹¹ | R ^{1a} | R ^{1b} | mp, °C |
|------------|-----------------|-----------------|---------------------------------|-----------------|---------------------------------|--|-----------|
| 1501 | CH ₂ | Cl | CF ₃ | H | C ₃ H ₇ | OCH ₃ | 76-78 |
| 1502 | CH ₂ | Cl | CF ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | oil |
| 1503 | CH ₂ | Cl | Cl | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1504 | CH ₂ | Cl | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1505 | CH ₂ | CF ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1506 | CH ₂ | Cl | SO ₂ CH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1507 | CH ₂ | Cl | COCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1508 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1509 | CH ₂ | Cl | CH ₃ | F | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1510 | CH ₂ | CH ₃ | OCH ₃ | F | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1511 | CH ₂ | CH ₃ | CH ₃ | CH ₃ | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1512 | CH ₂ | Cl | CF ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1513 | CH ₂ | Cl | Cl | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1514 | CH ₂ | Cl | OCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1515 | CH ₂ | CF ₃ | OCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1516 | CH ₂ | Cl | SO ₂ CH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1517 | CH ₂ | Cl | COCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1518 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1519 | CH ₂ | Cl | CH ₃ | F | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |

| | | | | | | | |
|------|-----------------|-----------------|---------------------------------|-----------------|---------------------------------|--|-----|
| 1520 | CH ₂ | CH ₃ | OCH ₃ | F | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1521 | CH ₂ | CH ₃ | CH ₃ | CH ₃ | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1522 | CH ₂ | Cl | CF ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | oil |
| 1523 | CH ₂ | Cl | Cl | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1524 | CH ₂ | Cl | OCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1525 | CH ₂ | CF ₃ | OCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1526 | CH ₂ | Cl | SO ₂ CH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1527 | CH ₂ | Cl | COCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1528 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1529 | CH ₂ | Cl | CH ₃ | F | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1530 | CH ₂ | CH ₃ | OCH ₃ | F | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1531 | CH ₂ | CH ₃ | CH ₃ | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1532 | CH ₂ | Cl | CF ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1533 | CH ₂ | Cl | Cl | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1534 | CH ₂ | Cl | OCH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1535 | CH ₂ | CF ₃ | OCH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1536 | CH ₂ | Cl | SO ₂ CH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1537 | CH ₂ | Cl | COCH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1538 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1539 | CH ₂ | Cl | CH ₃ | F | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1540 | CH ₂ | CH ₃ | OCH ₃ | F | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1541 | CH ₂ | CH ₃ | CH ₃ | CH ₃ | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1542 | O | Cl | CF ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | oil |
| 1543 | O | Cl | Cl | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1544 | O | Cl | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1545 | O | CF ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1546 | O | Cl | SO ₂ CH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1547 | O | Cl | COCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1548 | O | CH ₃ | OCH ₃ | CH ₃ | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1549 | O | Cl | CH ₃ | F | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1550 | O | CH ₃ | OCH ₃ | F | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1551 | O | CH ₃ | CH ₃ | CH ₃ | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1552 | O | Cl | CF ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1553 | O | Cl | Cl | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1554 | O | Cl | OCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1555 | O | CF ₃ | OCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1556 | O | Cl | SO ₂ CH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |

| | | | | | | | |
|------|---|-----------------|---------------------------------|-----------------|---------------------------------|--|-----|
| 1557 | 0 | Cl | COCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1558 | 0 | CH ₃ | OCH ₃ | CH ₃ | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1559 | 0 | Cl | CH ₃ | F | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1560 | 0 | CH ₃ | OCH ₃ | F | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1561 | 0 | CH ₃ | CH ₃ | CH ₃ | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1562 | 0 | Cl | CF ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | oil |
| 1563 | 0 | Cl | OCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1564 | 0 | CF ₃ | OCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1565 | 0 | Cl | SO ₂ CH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1566 | 0 | Cl | COCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1567 | 0 | CH ₃ | OCH ₃ | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1568 | 0 | Cl | CH ₃ | F | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1569 | 0 | CH ₃ | OCH ₃ | F | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1570 | 0 | CH ₃ | CH ₃ | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1571 | 0 | Cl | CF ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1572 | 0 | Cl | Cl | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1573 | 0 | Cl | OCH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1574 | 0 | CF ₃ | OCH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1575 | 0 | Cl | SO ₂ CH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1576 | 0 | Cl | COCH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1577 | 0 | CH ₃ | OCH ₃ | CH ₃ | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1578 | 0 | Cl | CH ₃ | F | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1579 | 0 | CH ₃ | OCH ₃ | F | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1580 | 0 | CH ₃ | CH ₃ | CH ₃ | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |

TABLE 1D

5



| Ex. No. | X | R ⁴ | R ⁵ | R ¹¹ | R ^{1a} | R ^{1b} | mp, °C |
|------------|-----------------|-----------------|---------------------------------|-----------------|---------------------------------|--|-----------|
| 1601 | CH ₂ | CH ₃ | Cl | H | C ₂ H ₅ | c-C ₃ H ₅ | 109-111 |
| 1602 | CH ₂ | Cl | Cl | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1603 | CH ₂ | Cl | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1604 | CH ₂ | CF ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1605 | CH ₂ | Cl | SO ₂ CH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1606 | CH ₂ | Cl | COCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1607 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1608 | CH ₂ | Cl | CH ₃ | F | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1609 | CH ₂ | CH ₃ | OCH ₃ | F | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1610 | CH ₂ | CH ₃ | CH ₃ | CH ₃ | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1611 | CH ₂ | Cl | CF ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1612 | CH ₂ | Cl | Cl | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1613 | CH ₂ | Cl | OCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1614 | CH ₂ | CF ₃ | OCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1615 | CH ₂ | Cl | SO ₂ CH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1616 | CH ₂ | Cl | COCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1617 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1618 | CH ₂ | Cl | CH ₃ | F | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1619 | CH ₂ | CH ₃ | OCH ₃ | F | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1620 | CH ₂ | CH ₃ | CH ₃ | CH ₃ | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1621 | CH ₂ | Cl | CF ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | oil |
| 1622 | CH ₂ | Cl | Cl | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1623 | CH ₂ | Cl | OCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1624 | CH ₂ | CF ₃ | OCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1625 | CH ₂ | Cl | SO ₂ CH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1626 | CH ₂ | Cl | COCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1627 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1628 | CH ₂ | Cl | CH ₃ | F | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1629 | CH ₂ | CH ₃ | OCH ₃ | F | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1630 | CH ₂ | CH ₃ | CH ₃ | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1631 | CH ₂ | Cl | CF ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1632 | CH ₂ | Cl | Cl | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1633 | CH ₂ | Cl | OCH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1634 | CH ₂ | CF ₃ | OCH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |

| | | | | | | | |
|------|-----------------|-----------------|---------------------------------|-----------------|---------------------------------|--|-----|
| 1635 | CH ₂ | Cl | SO ₂ CH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1636 | CH ₂ | Cl | COCH ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1637 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1638 | CH ₂ | Cl | CH ₃ | F | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1639 | CH ₂ | CH ₃ | OCH ₃ | F | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1640 | CH ₂ | CH ₃ | CH ₃ | CH ₃ | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |
| 1641 | O | Cl | CF ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | oil |
| 1642 | O | Cl | Cl | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1643 | O | Cl | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1644 | O | CF ₃ | OCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1645 | O | Cl | SO ₂ CH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1646 | O | Cl | COCH ₃ | H | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1647 | O | CH ₃ | OCH ₃ | CH ₃ | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1648 | O | Cl | CH ₃ | F | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1649 | O | CH ₃ | OCH ₃ | F | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1650 | O | CH ₃ | CH ₃ | CH ₃ | C ₂ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1651 | O | Cl | CF ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1652 | O | Cl | Cl | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1653 | O | Cl | OCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1654 | O | CF ₃ | OCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1655 | O | Cl | SO ₂ CH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1656 | O | Cl | COCH ₃ | H | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1657 | O | CH ₃ | OCH ₃ | CH ₃ | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1658 | O | Cl | CH ₃ | F | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1659 | O | CH ₃ | OCH ₃ | F | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1660 | O | CH ₃ | CH ₃ | CH ₃ | c-C ₃ H ₅ | C ₂ H ₄ OCH ₃ | - |
| 1661 | O | Cl | CF ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | oil |
| 1662 | O | Cl | OCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1663 | O | CF ₃ | OCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1664 | O | Cl | SO ₂ CH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1665 | O | Cl | COCH ₃ | H | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1666 | O | CH ₃ | OCH ₃ | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1667 | O | Cl | CH ₃ | F | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1668 | O | CH ₃ | OCH ₃ | F | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1669 | O | CH ₃ | CH ₃ | CH ₃ | C ₂ H ₅ | CH ₂ OCH ₃ | - |
| 1670 | O | Cl | CF ₃ | H | c-C ₃ H ₅ | CH ₂ OCH ₃ | - |

| | | | | | | | |
|------|---|-----------------|---------------------------------|-----------------|---------------------------------|----------------------------------|---|
| 1671 | O | Cl | Cl | H | c-C ₆ H ₅ | CH ₂ OCH ₃ | - |
| 1672 | O | Cl | OCH ₃ | H | c-C ₆ H ₅ | CH ₂ OCH ₃ | - |
| 1673 | O | CF ₃ | OCH ₃ | H | c-C ₆ H ₅ | CH ₂ OCH ₃ | - |
| 1674 | O | Cl | SO ₂ CH ₃ | H | c-C ₆ H ₅ | CH ₂ OCH ₃ | - |
| 1675 | O | Cl | COCH ₃ | H | c-C ₆ H ₅ | CH ₂ OCH ₃ | - |
| 1676 | O | CH ₃ | OCH ₃ | CH ₃ | c-C ₆ H ₅ | CH ₂ OCH ₃ | - |
| 1677 | O | Cl | CH ₃ | F | c-C ₆ H ₅ | CH ₂ OCH ₃ | - |
| 1678 | O | CH ₃ | OCH ₃ | F | c-C ₆ H ₅ | CH ₂ OCH ₃ | - |
| 1679 | O | CH ₃ | CH ₃ | CH ₃ | c-C ₆ H ₅ | CH ₂ OCH ₃ | - |

The methods discussed below in the preparation of 1-benzyl-6-methyl-4-(2,4,6-trimethylphenyl)imidazo[4,5-c]pyridine (Example 2001, Table 2, Structure A) may be used to prepare all of the examples of Structure A contained in Table 2, with minor procedural modifications where necessary and use of reagents of the appropriate structure.

10

The methods of Schemes 13 and 14 may be used to prepare many of the examples of Structure B and Structure C contained in Table 2, with minor procedural modifications where necessary and use of reagents of the appropriate structure.

15

Example 2001

Preparation of 1-benzyl-6-methyl-4-(2,4,6-trimethylphenyl)imidazo[4,5-c]pyridine

20

Part A. A solution of 4-chloro-6-methyl-3-nitropyridone (5.0 g, 26.5 mmol) in acetonitrile (93 mL) was treated with benzylamine (2.89 mL, 26.5 mmol) and diisopropylethylamine (5.54 mL, 31.8 mmol). The mixture was heated to reflux for 4 hrs., then cooled to ambient temperature and allowed to stir for 12 hrs. The mixture was partitioned between dichloromethane and water (200 mL each), and the aqueous layer was extracted with dichloromethane (200 mL). The

25

extracts were washed in sequence with water (200 mL) and combined, and the resulting precipitate was collected by filtration. The filtrate was dried over sodium sulfate, refiltered and evaporated to afford a second crop of

5 crystalline product, 4-benzylamino-6-methyl-3-nitropyridone (6.74 g total, 26.0 mmol, 98%). m.p. 246-247 °C. TLC R_f 0.35 (10:90 isopropanol-ethyl acetate). ^1H NMR (300 MHz, CDCl_3): d 10.48 (1H, br s), 9.69 (1H, br s), 7.41-7.26 (5H, m), 5.66 (1H, s), 4.57 (2H, d, $J = 5.5$ Hz), 2.26 (3H, s). MS

10 (NH_3 -CI): m/e 261 (10), 260 (70), 226 (100).

Part B. A solution of the pyridone from Part A (6.72 g, 25.9 mmol) in phosphorus oxychloride (52 mL, 25.5 mmol) was stirred at ambient temperature for 3 d. The reaction

15 mixture was poured into a mixture of ice (150 g) and dichloromethane (200 mL). After the ice had melted, 100 mL more dichloromethane was added, and the pH of the mixture was adjusted to 7 with solid NaHCO_3 . The mixture was separated, and the aqueous phase was extracted with

20 dichloromethane. The extracts were combined, dried over sodium sulfate, filtered and evaporated to afford the product (4-benzylamino-2-chloro-6-methyl-3-nitropyridine) as a bright yellow crystalline solid (6.45 g, 23.2 mmol, 90%). TLC R_f 0.76 (ethyl acetate). ^1H NMR (300 MHz, CDCl_3): d

25 7.43-7.26 (5H, m), 7.04 (1H, br), 6.47 (1H, s), 4.48 (2H, d, $J = 5.5$ Hz), 2.40 (3H, s). MS (NH_3 -CI): m/e 281 (5), 280 (35), 279 (17), 278 (100).

Part C. A solution of the nitro compound from Part B above

30 (6.42 g, 23.1 mmol) in methanol (162 mL) was treated with iron powder (13.61 g) and glacial acetic acid (13.6 mL). The resulting mixture was heated to reflux for 2 h, then cooled, filtered through celite (with methanol washing) and evaporated. The residual material was taken up in

35 dichloromethane (231 mL) and 1 N aq. HCl (162 mL), and adjusted to neutral pH by addition of solid NaHCO_3 . This mixture was filtered through celite and separated, and the aqueous phase was extracted with dichloromethane. The

- extracts were combined, dried over Na_2SO_4 , filtered and evaporated to afford the product, 3-amino-4-benzylamino-2-chloro-6-methylpyridine, as a solid (5.59 g, 22.6 mmol, 98%). m.p. 177-178 °C. TLC R_f 0.60 (ethyl acetate). ^1H NMR (300 MHz, CDCl_3): d 7.41-7.32 (5H, m), 6.33 (1H, s), 4.54 (1H, br), 4.36 (2H, d, $J = 5.1$ Hz), 3.30 (2H, br s), 2.35 (3H, s). MS (NH_3 -CI): m/e 251 (6), 250 (37), 249 (19), 248 (100).
- 10 Part D. A suspension of the diamine from Part C above (2.15 g, 8.68 mmol) in triethyl orthopropionate (5 mL) was treated with conc. HCl (3 drops), and heated to reflux for 1 h, then cooled and the excess orthoester removed by vacuum distillation. The pot residue was taken up in ethyl acetate (120 mL), which was washed with water and brine (100 mL each). The aqueous phases were back-extracted in sequence with ethyl acetate, and the extracts were combined, dried over Na_2SO_4 , filtered and evaporated to afford N-(4-benzylamino-2-chloro-6-methylpyridin-3-yl)propionamide O-ethyl imidate (2.62 g, 91%). TLC R_f 0.40 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): d 7.39-7.29 (5H, m), 6.29 (1H, s), 4.64 (1H, br t, $J = 5.8$ Hz), 4.37 (2H, d, $J = 5.8$ Hz), 4.25 (2H, br), 2.35 (3H, s), 2.18-2.11 (2H, m), 1.36 (3H, t, $J = 7.0$ Hz), 1.06 (3H, t, $J = 7.7$ Hz). MS (NH_3 -CI): m/e 335 (7), 334 (34), 333 (22), 332 (100).

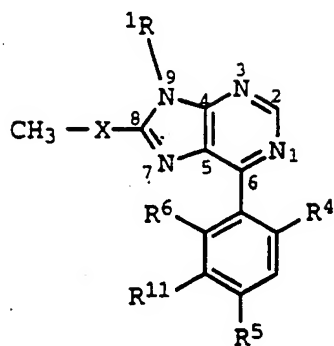
- Part E. A solution of the compound from Part D (2.62 g, 7.90 mmol) in phenyl ether (10 mL) was heated to 170 °C for 6 h, then cooled and poured into ethyl acetate (150 mL). This was washed with water and brine (100 mL each), then dried over Na_2SO_4 , filtered and evaporated. The residual liquid was separated by column chromatography (hexane, then ethyl acetate) to afford the product, 1-benzyl-4-chloro-2-ethyl-6-methylimidazo[4,5-c]pyridine, as an oil (2.16 g, 96%). m.p. 140-141 °C. TLC R_f 0.06 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): d 7.36-7.32 (3H, m), 7.02-6.98 (2H, m), 6.93 (1H, s), 5.31 (2H, s), 2.89 (2H, q, $J =$

7.3 Hz), 2.58 (3H, s), 1.39 (3H, t, $J = 7.3$ Hz). MS (NH_3 -CI): m/e 289 (6), 288 (35), 287 (20), 286 (100).

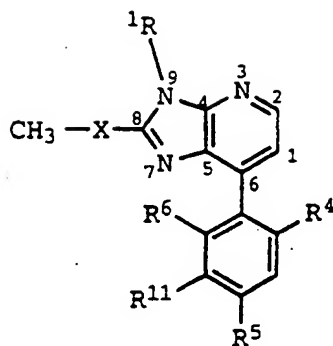
Part F. A solution of zinc chloride (538 mg) in
5 tetrahydrofuran (7 mL) was treated with a tetrahydrofuran
solution of 2-mesitylmagnesium bromide (3.95 mL, 1.0 M), and
stirred for 1 h. In another flask, a solution of
bis(triphenylphosphine)palladium chloride (93 mg, 0.132 mmol)
in tetrahydrofuran (5 mL) was treated with a hexane solution
10 of diisobutylaluminum hydride (0.263 mL, 1.0 M), and this
solution was stirred for 20 min. The arylzinc solution was
then delivered by cannula to the flask containing the
palladium catalyst, which was followed by the chloride
prepared in Part E. The mixture was heated to reflux for 12 h,
15 then cooled, and poured into water (100 mL). This was
extracted with ethyl acetate (2 x 150 mL), and the extracts
were washed with brine, combined, dried over Na_2SO_4 , filtered
and evaporated. The residual material was separated by column
chromatography (1:1 ethyl acetate-hexane) to afford the title
20 product as a solid, recrystallized to purity from ether (187
mg, 29%). m.p. 177-180 °C (ether). TLC R_f 0.27 (50:50 ethyl
acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 7.38-7.32 (3H, m),
7.10-7.05 (2H, m), 6.96 (1H, s), 6.93 (2H, s), 5.32 (2H, s),
2.84 (2H, q, $J = 7.3$ Hz), 2.64 (3H, s), 2.30 (3H, s), 2.02
25 (6H, s), 1.26 (3H, t, $J = 7.3$ Hz). MS (NH_3 -CI): m/e 372 (4),
371 (29), 370 (100). Analysis calc'd for $\text{C}_{25}\text{H}_{27}\text{N}_3$: C, 81.26; H,
7.38; N, 11.37; found: C, 80.70; H, 7.26; N, 11.20.

30

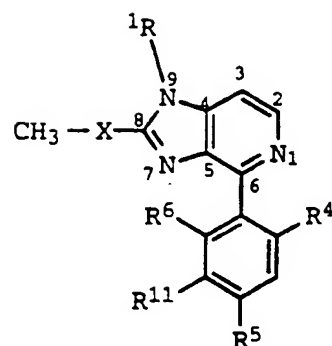
TABLE 2



(A)



(B)



(C)

| Ex. No. | X | R ⁴ | R ⁵ | R ¹¹ | R ⁶ | R ¹ | mp, °C |
|---------|-----------------|----------------|-----------------|-----------------|----------------|---|-----------|
| 2001 | CH ₂ | Cl | Cl | H | H | c-C ₄ H ₇ | - |
| 2002 | CH ₂ | Cl | Cl | H | H | c-C ₅ H ₉ | 111-112 |
| 2003 | CH ₂ | Cl | Cl | H | H | c-C ₆ H ₁₁ | oil |
| 2004 | CH ₂ | Cl | Cl | H | H | c-C ₇ H ₁₃ | 128-130 |
| 2005 | CH ₂ | Cl | Cl | H | H | c-C ₈ H ₁₅ | - |
| 2006 | CH ₂ | Cl | Cl | H | H | 2-CH ₃ -c-C ₅ H ₈ | oil |
| 2007 | CH ₂ | Cl | Cl | H | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2008 | CH ₂ | Cl | Cl | H | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2009 | CH ₂ | Cl | Cl | H | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2010 | CH ₂ | Cl | Cl | H | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2011 | CH ₂ | Cl | Cl | H | H | 9-fluorenyl | oil |
| 2012 | CH ₂ | Cl | Cl | H | H | 1-tetrahydronaphthyl | oil |
| 2013 | CH ₂ | Cl | Cl | H | H | 1-indanyl | oil |
| 2014 | CH ₂ | Cl | Cl | H | H | 4-chromanyl | oil |
| 2015 | CH ₂ | Cl | Cl | H | H | 2-oxo-c-C ₅ H ₇ | 166-168 |
| 2016 | CH ₂ | Cl | Cl | H | H | 5-dibenzosuberyl | - |
| 2017 | CH ₂ | Cl | Cl | H | H | 5-dibenzosubereryl | - |
| 2018 | CH ₂ | Cl | CF ₃ | H | H | c-C ₄ H ₇ | - |
| 2019 | CH ₂ | Cl | CF ₃ | H | H | c-C ₅ H ₉ | 146-147 |
| 2020 | CH ₂ | Cl | CF ₃ | H | H | c-C ₆ H ₁₁ | oil |
| 2021 | CH ₂ | Cl | CF ₃ | H | H | c-C ₇ H ₁₃ | 129-130 |
| 2022 | CH ₂ | Cl | CF ₃ | H | H | c-C ₈ H ₁₅ | - |
| 2023 | CH ₂ | Cl | CF ₃ | H | H | 2-CH ₃ -c-C ₅ H ₈ | 98-99 |

| | | | | | | | |
|------|-----------------|----|------------------|---|---|---|-----|
| 2024 | CH ₂ | Cl | CF ₃ | H | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2025 | CH ₂ | Cl | CF ₃ | H | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2026 | CH ₂ | Cl | CF ₃ | H | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2027 | CH ₂ | Cl | CF ₃ | H | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2028 | CH ₂ | Cl | CF ₃ | H | H | 9-fluorenyl | - |
| 2029 | CH ₂ | Cl | CF ₃ | H | H | 1-tetrahydronaphthyl | - |
| 2030 | CH ₂ | Cl | CF ₃ | H | H | 1-indanyl | - |
| 2031 | CH ₂ | Cl | CF ₃ | H | H | 4-chromanyl | - |
| 2032 | CH ₂ | Cl | CF ₃ | H | H | 2-oxo-c-C ₅ H ₇ | - |
| 2033 | CH ₂ | Cl | CF ₃ | H | H | 5-dibenzosuberyl | - |
| 2034 | CH ₂ | Cl | CF ₃ | H | H | 5-dibenzosubereryl | - |
| 2035 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₄ H ₇ | - |
| 2036 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₅ H ₉ | - |
| 2037 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₆ H ₁₁ | - |
| 2038 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₇ H ₁₃ | - |
| 2039 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₈ H ₁₅ | - |
| 2040 | CH ₂ | Cl | OCH ₃ | H | H | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2041 | CH ₂ | Cl | OCH ₃ | H | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2042 | CH ₂ | Cl | OCH ₃ | H | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2043 | CH ₂ | Cl | OCH ₃ | H | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2044 | CH ₂ | Cl | OCH ₃ | H | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2045 | CH ₂ | Cl | OCH ₃ | H | H | 9-fluorenyl | - |
| 2046 | CH ₂ | Cl | OCH ₃ | H | H | 1-tetrahydronaphthyl | - |
| 2047 | CH ₂ | Cl | OCH ₃ | H | H | 1-indanyl | - |
| 2048 | CH ₂ | Cl | OCH ₃ | H | H | 4-chromanyl | - |
| 2049 | CH ₂ | Cl | OCH ₃ | H | H | 2-oxo-c-C ₅ H ₇ | - |
| 2050 | CH ₂ | Cl | OCH ₃ | H | H | 5-dibenzosuberyl | - |
| 2051 | CH ₂ | Cl | OCH ₃ | H | H | 5-dibenzosubereryl | - |
| 2052 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₄ H ₇ | - |
| 2053 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₅ H ₉ | oil |
| 2054 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₆ H ₁₁ | - |
| 2055 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₇ H ₁₃ | - |
| 2056 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₈ H ₁₅ | - |
| 2057 | CH ₂ | Cl | OCF ₃ | H | H | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2058 | CH ₂ | Cl | OCF ₃ | H | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2059 | CH ₂ | Cl | OCF ₃ | H | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2060 | CH ₂ | Cl | OCF ₃ | H | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2061 | CH ₂ | Cl | OCF ₃ | H | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |

| | | | | | | | |
|------|-----------------|-----------------|------------------|---|---|---|---------|
| 2062 | CH ₂ | Cl | OCF ₃ | H | H | 9-fluorenyl | - |
| 2063 | CH ₂ | Cl | OCF ₃ | H | H | 1-tetrahydronaphthyl | - |
| 2064 | CH ₂ | Cl | OCF ₃ | H | H | 1-indanyl | - |
| 2065 | CH ₂ | Cl | OCF ₃ | H | H | 4-chromanyl | - |
| 2066 | CH ₂ | Cl | OCF ₃ | H | H | 2-oxo-c-C ₅ H ₇ | - |
| 2067 | CH ₂ | Cl | OCF ₃ | H | H | 5-dibenzosuberyl | - |
| 2068 | CH ₂ | Cl | OCF ₃ | H | H | 5-dibenzosubereryl | - |
| 2069 | CH ₂ | Cl | CH ₃ | H | H | c-C ₄ H ₇ | - |
| 2070 | CH ₂ | Cl | CH ₃ | H | H | c-C ₅ H ₉ | - |
| 2071 | CH ₂ | Cl | CH ₃ | H | H | c-C ₆ H ₁₁ | - |
| 2072 | CH ₂ | Cl | CH ₃ | H | H | c-C ₇ H ₁₃ | - |
| 2073 | CH ₂ | Cl | CH ₃ | H | H | c-C ₈ H ₁₅ | - |
| 2074 | CH ₂ | Cl | CH ₃ | H | H | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2075 | CH ₂ | Cl | CH ₃ | H | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2076 | CH ₂ | Cl | CH ₃ | H | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2077 | CH ₂ | Cl | CH ₃ | H | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2078 | CH ₂ | Cl | CH ₃ | H | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2079 | CH ₂ | Cl | CH ₃ | H | H | 9-fluorenyl | - |
| 2080 | CH ₂ | Cl | CH ₃ | H | H | 1-tetrahydronaphthyl | - |
| 2081 | CH ₂ | Cl | CH ₃ | H | H | 1-indanyl | - |
| 2082 | CH ₂ | Cl | CH ₃ | H | H | 4-chromanyl | - |
| 2083 | CH ₂ | Cl | CH ₃ | H | H | 2-oxo-c-C ₅ H ₇ | - |
| 2084 | CH ₂ | Cl | CH ₃ | H | H | 5-dibenzosuberyl | - |
| 2085 | CH ₂ | Cl | CH ₃ | H | H | 5-dibenzosubereryl | - |
| 2086 | CH ₂ | CF ₃ | Cl | H | H | c-C ₄ H ₇ | - |
| 2087 | CH ₂ | CF ₃ | Cl | H | H | c-C ₅ H ₉ | 143-145 |
| 2088 | CH ₂ | CF ₃ | Cl | H | H | c-C ₆ H ₁₁ | - |
| 2089 | CH ₂ | CF ₃ | Cl | H | H | c-C ₇ H ₁₃ | - |
| 2090 | CH ₂ | CF ₃ | Cl | H | H | c-C ₈ H ₁₅ | - |
| 2091 | CH ₂ | CF ₃ | Cl | H | H | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2092 | CH ₂ | CF ₃ | Cl | H | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2093 | CH ₂ | CF ₃ | Cl | H | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2094 | CH ₂ | CF ₃ | Cl | H | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2095 | CH ₂ | CF ₃ | Cl | H | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2096 | CH ₂ | CF ₃ | Cl | H | H | 9-fluorenyl | - |
| 2097 | CH ₂ | CF ₃ | Cl | H | H | 1-tetrahydronaphthyl | - |
| 2098 | CH ₂ | CF ₃ | Cl | H | H | 1-indanyl | - |
| 2099 | CH ₂ | CF ₃ | Cl | H | H | 4-chromanyl | - |

| | | | | | | | |
|------|-----------------|-----------------|------------------|-----------------|---|---|---------|
| 2100 | CH ₂ | CF ₃ | Cl | H | H | 2-oxo-c-C ₅ H ₇ | - |
| 2101 | CH ₂ | CF ₃ | Cl | H | H | 5-dibenzosuberyl | - |
| 2102 | CH ₂ | CF ₃ | Cl | H | H | 5-dibenzosubereryl | - |
| 2103 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₄ H ₇ | - |
| 2104 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₅ H ₉ | 103-106 |
| 2105 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₆ H ₁₁ | - |
| 2106 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₇ H ₁₃ | - |
| 2107 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₈ H ₁₅ | - |
| 2108 | CH ₂ | CF ₃ | OCH ₃ | H | H | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2109 | CH ₂ | CF ₃ | OCH ₃ | H | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2110 | CH ₂ | CF ₃ | OCH ₃ | H | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2111 | CH ₂ | CF ₃ | OCH ₃ | H | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2112 | CH ₂ | CF ₃ | OCH ₃ | H | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2113 | CH ₂ | CF ₃ | OCH ₃ | H | H | 9-fluorenyl | - |
| 2114 | CH ₂ | CF ₃ | OCH ₃ | H | H | 1-tetrahydronaphthyl | - |
| 2115 | CH ₂ | CF ₃ | OCH ₃ | H | H | 1-indanyl | - |
| 2116 | CH ₂ | CF ₃ | OCH ₃ | H | H | 4-chromanyl | - |
| 2117 | CH ₂ | CF ₃ | OCH ₃ | H | H | 2-oxo-c-C ₅ H ₇ | - |
| 2118 | CH ₂ | CF ₃ | OCH ₃ | H | H | 5-dibenzosuberyl | - |
| 2119 | CH ₂ | CF ₃ | OCH ₃ | H | H | 5-dibenzosubereryl | - |
| 2120 | CH ₂ | CF ₃ | F | H | H | c-C ₄ H ₇ | - |
| 2121 | CH ₂ | CF ₃ | F | H | H | c-C ₅ H ₉ | - |
| 2122 | CH ₂ | CF ₃ | F | H | H | c-C ₆ H ₁₁ | - |
| 2123 | CH ₂ | CF ₃ | F | H | H | c-C ₇ H ₁₃ | 119-122 |
| 2124 | CH ₂ | CF ₃ | F | H | H | c-C ₈ H ₁₅ | - |
| 2125 | CH ₂ | CF ₃ | F | H | H | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2126 | CH ₂ | CF ₃ | F | H | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2127 | CH ₂ | CF ₃ | F | H | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2128 | CH ₂ | CF ₃ | F | H | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2129 | CH ₂ | CF ₃ | F | H | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | 155-156 |
| 2130 | CH ₂ | CF ₃ | F | H | H | 9-fluorenyl | 184-185 |
| 2131 | CH ₂ | CF ₃ | F | H | H | 1-tetrahydronaphthyl | - |
| 2132 | CH ₂ | CF ₃ | F | H | H | 1-indanyl | - |
| 2133 | CH ₂ | CF ₃ | F | H | H | 4-chromanyl | - |
| 2134 | CH ₂ | CF ₃ | F | H | H | 2-oxo-c-C ₅ H ₇ | - |
| 2135 | CH ₂ | CF ₃ | F | H | H | 5-dibenzosuberyl | - |
| 2136 | CH ₂ | CF ₃ | F | H | H | 5-dibenzosubereryl | - |
| 2137 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₄ H ₇ | - |

| | | | | | | | |
|------|-----------------|-----------------|------------------|-----------------|---|---|---------|
| 2138 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₅ H ₉ | - |
| 2139 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₆ H ₁₁ | - |
| 2140 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₇ H ₁₃ | - |
| 2141 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₈ H ₁₅ | - |
| 2142 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2143 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2144 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2145 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2146 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2147 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 9-fluorenyl | - |
| 2148 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 1-tetrahydronaphthyl | - |
| 2149 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 1-indanyl | - |
| 2150 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 4-chromanyl | - |
| 2151 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 2-oxo-c-C ₅ H ₇ | - |
| 2152 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 5-dibenzosuberyl | - |
| 2153 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | 5-dibenzosubereryl | - |
| 2154 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₄ H ₇ | - |
| 2155 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₅ H ₉ | 115-116 |
| 2156 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₆ H ₁₁ | - |
| 2157 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₇ H ₁₃ | - |
| 2158 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₈ H ₁₅ | - |
| 2159 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2160 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2161 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2162 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2163 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2164 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 9-fluorenyl | - |
| 2165 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 1-tetrahydronaphthyl | - |
| 2166 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 1-indanyl | - |
| 2167 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 4-chromanyl | - |
| 2168 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 2-oxo-c-C ₅ H ₇ | - |
| 2169 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 5-dibenzosuberyl | - |
| 2170 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | 5-dibenzosubereryl | - |
| 2171 | CH ₂ | CH ₃ | OCH ₃ | F | H | c-C ₄ H ₇ | - |
| 2172 | CH ₂ | CH ₃ | OCH ₃ | F | H | c-C ₅ H ₉ | - |
| 2173 | CH ₂ | CH ₃ | OCH ₃ | F | H | c-C ₆ H ₁₁ | - |
| 2174 | CH ₂ | CH ₃ | OCH ₃ | F | H | c-C ₇ H ₁₃ | - |
| 2175 | CH ₂ | CH ₃ | OCH ₃ | F | H | c-C ₈ H ₁₅ | - |

| | | | | | | | |
|------|-----------------|-----------------|------------------|---|-----------------|---|---|
| 2176 | CH ₂ | CH ₃ | OCH ₃ | F | H | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2177 | CH ₂ | CH ₃ | OCH ₃ | F | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2178 | CH ₂ | CH ₃ | OCH ₃ | F | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2179 | CH ₂ | CH ₃ | OCH ₃ | F | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2180 | CH ₂ | CH ₃ | OCH ₃ | F | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2181 | CH ₂ | CH ₃ | OCH ₃ | F | H | 9-fluorenyl | - |
| 2182 | CH ₂ | CH ₃ | OCH ₃ | F | H | 1-tetrahydronaphthyl | - |
| 2183 | CH ₂ | CH ₃ | OCH ₃ | F | H | 1-indanyl | - |
| 2184 | CH ₂ | CH ₃ | OCH ₃ | F | H | 4-chromanyl | - |
| 2185 | CH ₂ | CH ₃ | OCH ₃ | F | H | 2-oxo-c-C ₅ H ₇ | - |
| 2186 | CH ₂ | CH ₃ | OCH ₃ | F | H | 5-dibenzosuberyl | - |
| 2187 | CH ₂ | CH ₃ | OCH ₃ | F | H | 5-dibenzosubereryl | - |
| 2188 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₄ H ₇ | - |
| 2189 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₅ H ₉ | - |
| 2190 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₆ H ₁₁ | - |
| 2191 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₇ H ₁₃ | - |
| 2192 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₈ H ₁₅ | - |
| 2193 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2194 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2195 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2196 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2197 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2198 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 9-fluorenyl | - |
| 2199 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 1-tetrahydronaphthyl | - |
| 2200 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 1-indanyl | - |
| 2201 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 4-chromanyl | - |
| 2202 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 2-oxo-c-C ₅ H ₇ | - |
| 2203 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 5-dibenzosuberyl | - |
| 2204 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | 5-dibenzosubereryl | - |
| 2205 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₄ H ₇ | - |
| 2206 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₅ H ₉ | - |
| 2207 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₆ H ₁₁ | - |
| 2208 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₇ H ₁₃ | - |
| 2209 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₈ H ₁₅ | - |
| 2210 | CH ₂ | Cl | Cl | H | CH ₃ | 2-CH ₃ -c-C ₅ H ₈ | - |
| 2211 | CH ₂ | Cl | Cl | H | CH ₃ | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2212 | CH ₂ | Cl | Cl | H | CH ₃ | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2213 | CH ₂ | Cl | Cl | H | CH ₃ | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |

| | | | | | | | |
|------|-----------------|-----------------|------------------|------------------|-----------------|---|-----|
| 2214 | CH ₂ | Cl | Cl | H | CH ₃ | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2215 | CH ₂ | Cl | Cl | H | CH ₃ | 9-fluorenyl | - |
| 2216 | CH ₂ | Cl | Cl | H | CH ₃ | 1-tetrahydronaphthyl | oil |
| 2217 | CH ₂ | Cl | Cl | H | CH ₃ | 1-indanyl | - |
| 2218 | CH ₂ | Cl | Cl | H | CH ₃ | 4-chromanyl | - |
| 2219 | CH ₂ | Cl | Cl | H | CH ₃ | 2-oxo-c-C ₅ H ₇ | - |
| 2220 | CH ₂ | Cl | Cl | H | CH ₃ | 5-dibenzosuberyl | - |
| 2221 | CH ₂ | Cl | Cl | H | CH ₃ | 5-dibenzosubereryl | - |
| 2222 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | c-C ₄ H ₇ | - |
| 2223 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | c-C ₅ H ₉ | oil |
| 2224 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | c-C ₆ H ₁₁ | - |
| 2225 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | c-C ₇ H ₁₃ | - |
| 2226 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | c-C ₈ H ₁₅ | - |
| 2227 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 2-CH ₃ -c-C ₅ H ₈ | oil |
| 2228 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 3-CH ₃ -c-C ₅ H ₈ | - |
| 2229 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 2-OCH ₃ -c-C ₅ H ₈ | - |
| 2230 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 2,5-(CH ₃) ₂ -c-C ₅ H ₇ | - |
| 2231 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 2-(CH ₃) ₂ CH-5-CH ₃ -c-C ₆ H ₉ | - |
| 2232 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 9-fluorenyl | - |
| 2233 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 1-tetrahydronaphthyl | - |
| 2234 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 1-indanyl | - |
| 2235 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 4-chromanyl | - |
| 2236 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 2-oxo-c-C ₅ H ₇ | - |
| 2237 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 5-dibenzosuberyl | - |
| 2238 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | 5-dibenzosubereryl | - |
| 2239 | O | Cl | Cl | H | H | c-C ₅ H ₉ | - |
| 2240 | O | Cl | CF ₃ | H | H | c-C ₅ H ₉ | - |
| 2241 | O | Cl | OCH ₃ | H | H | c-C ₅ H ₉ | - |
| 2242 | O | Cl | OCF ₃ | H | H | c-C ₅ H ₉ | - |
| 2243 | O | Cl | CH ₃ | H | H | c-C ₅ H ₉ | - |
| 2244 | O | CF ₃ | Cl | H | H | c-C ₅ H ₉ | - |
| 2245 | O | CF ₃ | OCH ₃ | H | H | c-C ₅ H ₉ | - |
| 2246 | O | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₅ H ₉ | - |
| 2247 | O | CH ₃ | OCH ₃ | Cl | H | c-C ₅ H ₉ | - |
| 2248 | O | CH ₃ | OCH ₃ | F | H | c-C ₅ H ₉ | - |
| 2249 | O | CH ₃ | CH ₃ | H | CH ₃ | c-C ₅ H ₉ | - |
| 2250 | O | Cl | Cl | H | CH ₃ | c-C ₅ H ₉ | - |

Key:

a) Where the compound is listed as an "oil", spectral data is as follows:

Example 2003 spectral data: MS ($\text{NH}_3\text{-Cl}$): m/e 374 ($\text{M}+\text{H}^+$, 100%).

- 5 Example 2006 spectral data: TLC R_f 0.20 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.94 (1H, s), 7.67 (1H, d, J = 8.1 Hz), 7.57 (1H, d, J = 1.8 Hz), 7.40 (1H, dd, J = 8.1, 1.8 Hz), 4.83 (1H, q, J = 8.0 Hz), 3.20-3.04 (1H, m), 2.98 (2H, q, J = 7.3 Hz), 2.50-2.38 (1H, m), 2.30-2.15 (2H, m), 2.03-1.93 (2H, m), 1.75-1.60 (1H, m), 1.42 (3H, t, J = 7.3 Hz), 0.68 (3H, d, J = 6.9 Hz). MS ($\text{NH}_3\text{-Cl}$): m/e calc'd for $\text{C}_{19}\text{H}_{21}\text{Cl}_2\text{N}_4$: 375.1143, found 375.1149; 380 (2), 379 (12), 378 (15), 377 (66), 376 (27), 375 (100).

Example 2011 spectral data: MS ($\text{NH}_3\text{-Cl}$): m/e 457 ($\text{M}+\text{H}^+$, 100%).

- 15 Example 2012 spectral data: TLC R_f 0.38 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.94 (1H, s), 7.72 (1H, d, J = 8.5 Hz), 7.58 (1H, d, J = 1.8 Hz), 7.47-7.40 (2H, m), 7.24-7.18 (1H, m), 6.56 (1H, d, J = 7.7 Hz), 6.18-6.10 (1H, m), 4.82-4.76 (1H, m), 3.15-2.30 (5H, m), 2.10-1.77 (3H, m), 1.27 (3H, t, J = 7.5 Hz). MS ($\text{NH}_3\text{-Cl}$): m/e calc'd for $\text{C}_{23}\text{H}_{21}\text{Cl}_2\text{N}_4$: 423.1143, found 423.1142; 427 (13), 426 (18), 425 (67), 424 (31), 423 (100).

- 20 Example 2013 spectral data: TLC R_f 0.28 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.91 (1H, s), 7.68 (1H, d, J = 8.5 Hz), 7.58 (1H, d, J = 1.8 Hz), 7.46-7.38 (2H, m), 7.22-7.15 (1H, m), 6.91 (1H, d, J = 7.7 Hz), 6.42 (1H, br t, J = 7 Hz), 5.30-5.22 (1H, m), 3.43-3.33 (1H, m), 3.20-3.03 (1H, m), 2.89-2.76 (2H, m), 2.56-2.43 (1H, m), 2.01-1.90 (1H, m), 1.31 (3H, t, J = 7.5 Hz). MS ($\text{NH}_3\text{-Cl}$): m/e calc'd for $\text{C}_{22}\text{H}_{19}\text{Cl}_2\text{N}_4$: 409.0987, found 409.0987; 413 (12), 412 (17), 411 (67), 410 (29), 409 (100).

- 30 Example 2014 spectral data: TLC R_f 0.38 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.95 (1H, s), 7.71 (1H, d, J = 8.4 Hz), 7.59 (1H, d, J = 2.2 Hz), 7.42 (1H, dd, J = 8.4, 2.2 Hz), 7.26-7.19 (1H, m), 6.98-6.90 (1H, m), 6.58 (1H, d, J = 7.7 Hz), 6.30-6.22 (1H, m), 4.60-4.53 (1H, m), 4.43-4.33 (1H, m), 4.20 (1H, br), 2.82-2.72 (1H, m), 2.69-2.58 (1H, m), 2.46-2.36 (1H, m), 2.18-2.08 (1H, m), 1.29 (3H, t, J = 7.5 Hz). MS ($\text{NH}_3\text{-Cl}$): m/e calc'd for $\text{C}_{22}\text{H}_{19}\text{Cl}_2\text{N}_4\text{O}$: 425.0936, found 425.0926; 429 (12), 428 (17), 427 (67), 426 (30), 425 (100).

- 35 Example 2020 spectral data: TLC R_f 0.43 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.98 (1H, s), 7.81 (2H, d, J = 8.4 Hz), 7.67 (1H,

dd, $J = 8.0, 0.7$ Hz), 4.26 (1H, m), 3.00 (2H, q, $J = 7.6$ Hz), 2.75-2.66 (2H, m), 2.06-1.90 (4H, m), 1.50-1.36 (4H, m), 1.40 (3H, t, $J = 7.5$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e 412 (7), 411 (34), 410 (25), 409 (100).

Example 2053 spectral data: TLC R_f 0.36 (25:75 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.96 (1H, s), 7.73 (1H, d, $J = 8.4$ Hz), 7.44 (1H, d, $J = 1.1$ Hz), 7.28 (1H, dd, $J = 8.4, 1.1$ Hz), 4.79 (1H, pentet, $J = 8.4$ Hz), 3.01 (2H, q, $J = 7.7$ Hz), 2.62-2.50 (2H, m), 2.23-2.07 (2H, m), 1.89-1.77 (2H, m), 1.66-1.49 (2H, m), 1.41 (3H, t, $J = 7.7$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{11}\text{H}_{13}\text{ClF}_3\text{N}_4\text{O}$: 411.1205, found 411.1208; 414 (7), 413 (34), 412 (24), 411 (100).

Example 2216 spectral data: TLC R_f 0.13 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.94 (1H, s), 7.48-7.02 (5H, m), 6.53 (1H, dd, $J = 7.7, 1.5$ Hz), 6.18-6.10 (1H, m), 3.16-2.20 (5H, m), 2.13 (3H, d, $J = 4.8$ Hz), 2.06-1.70 (3H, m), 1.23 (3H, dt, $J = 7.4, 4.4$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{24}\text{H}_{23}\text{Cl}_2\text{N}_4$: 437.1300, found 437.1299; 439 (67), 437 (100).

Example 2223 spectral data: TLC R_f 0.36 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.91 (1H, s), 7.33 (1H, s), 6.83 (1H, s), 4.78 (1H, pentet, $J = 8.5$ Hz), 3.94 (3H, s), 3.90 (3H, s), 2.98 (2H, q, $J = 7.6$ Hz), 2.58-2.48 (2H, m), 2.42 (3H, s), 2.19-2.07 (2H, m), 1.84-1.56 (4H, m), 1.43 (3H, t, $J = 7.5$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{21}\text{H}_{27}\text{N}_4\text{O}_2$: 367.2134, found 367.2120; 369 (3), 368 (24), 367 (100).

Example 2227 spectral data: TLC R_f 0.45 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.90 (1H, s), 7.37 (1H, s), 6.83 (1H, s), 4.85 (1H, q, $J = 8.4$ Hz), 3.94 (3H, s), 3.91 (3H, s), 3.19-3.11 (1H, m), 2.96 (2H, dq, $J = 7.9, 1.5$ Hz), 2.41 (3H, s), 2.24-2.16 (2H, m), 2.04-1.94 (2H, m), 1.71-1.62 (2H, m), 1.44 (3H, t, $J = 7.4$ Hz), 0.69 (3H, d, $J = 6.9$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{22}\text{H}_{29}\text{N}_4\text{O}_2$: 381.2290, found 381.2294; 383 (4), 382 (25), 381 (100).

30

The methods discussed below in the preparation of 3-benzyl-5-methyl-7-(2,4,6-trimethylphenyl)-imidazo[4,5-b]pyridine (Example 3001, Table 3) may be used to prepare all of the examples of Structure A contained in Table 3, with minor procedural modifications where necessary and use of reagents of the appropriate structure.

35

The methods of Schemes 13 and 14 may be used to prepare many of the examples of Structure B and Structure C contained in Table 3, with minor procedural modifications where necessary and use of reagents of the appropriate structure.

Example 3001

Preparation of 3-benzyl-5-methyl-7-(2,4,6-trimethylphenyl)imidazo[4,5-b]pyridine

Part A. A solution of 2,4,6-trimethylbenzeneboronic acid in benzene (0.5 M) is treated with excess *n*-butanol, and the solution is heated to reflux under a Dean-Stark still head to azeotropically remove water. Solvent is removed by evaporation, and the resulting dibutyl 2,4,6-trimethylbenzeneboronate is used directly in Part B.

Part B. The method of Snieckus et al. (Fu, J. M.; Zhao, B. P.; Sharp, M. J.; Snieckus, V. *Can. J. Chem.* **1994**, 72, 227-236) may be employed here. Thus, a solution of 4-chloro-6-methyl-3-nitro-2-pyridone in dimethylformamide (0.1 M) is treated with the boronate from Part A (1.2 eq), tribasic potassium phosphate (2.4 eq), and [1,1'-bis(diphenylphosphino)-ferrocene]dichloropalladium (0.1 eq). The mixture is stirred at ambient temperature for 30 hrs., then poured into 4 volumes ethyl acetate. This is washed with 3 equal volumes of water, then brine. The extract is dried over Na_2SO_4 , filtered and evaporated. Chromatographic separation affords pure 6-methyl-3-nitro-4-(2,4,6-trimethylphenyl)-2-pyridone.

Part C. The pyridone from Part B is suspended in 6 eq phosphorus oxychloride, and stirred with mild heating until the compound dissolves. The mixture is cooled, and poured over ice. After melting, the mixture is extracted twice with dichloromethane, and the extracts are combined, dried over Na_2SO_4 , filtered and evaporated. The product, 2-chloro-

6-methyl-3-nitro-4-(2,4,6-trimethylphenyl)pyridine, is purified by either chromatography or recrystallization.

Part D. The chloride from Part C is dissolved in ethanol, and treated with benzylamine (1.2 eq.). The mixture is heated to reflux until the starting material is consumed as determined by thin-layer chromatography. The mixture is evaporated, and the residual material is partitioned between water and ethyl acetate. The organic layer is separated, washed with brine, dried over Na_2SO_4 , filtered and evaporated. The product, 2-benzylamino-6-methyl-3-nitro-4-(2,4,6-trimethylphenyl)pyridine, is purified by either chromatography or recrystallization.

Part E. The nitro compound from Part D is dissolved in 1:1 aqueous dioxane, and treated with conc. aq. ammonium hydroxide solution. To this is added solid sodium dithionite in several portions over 2 h. The mixture is allowed to stir for an additional 4 h, then partitioned between water and ethyl acetate. The organic layer is separated, washed with brine, dried over Na_2SO_4 , filtered and evaporated. The product, 3-amino-2-benzylamino-6-methyl-4-(2,4,6-trimethylphenyl)pyridine, is purified by either chromatography or recrystallization.

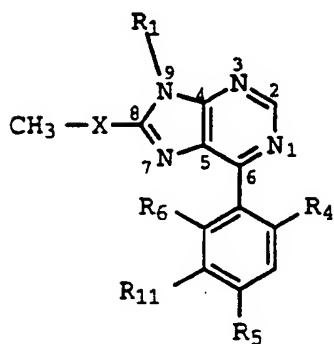
Part F. A suspension of the diamine from Part E above in triethyl orthopropionate is treated with conc. HCl , and heated to reflux for 1 h, then cooled and the excess orthoester removed by vacuum distillation. The pot residue contains sufficiently pure N-[2-benzylamino-4-(2,4,6-trimethylphenyl)-6-methylpyridin-3-yl]propionamide O-ethyl imidate.

Part G. A solution of the compound from Part F in phenyl ether is treated with a catalytic amount of p-toluenesulfonic acid and heated to 170°C for 6 h, then cooled. The residual liquid is separated by column

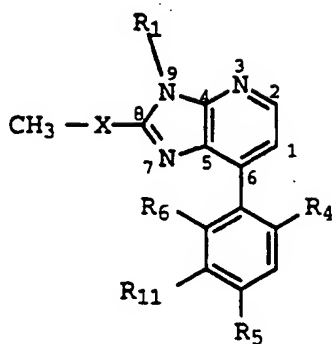
chromatography (hexane, then ethyl acetate) to afford the title product.

5

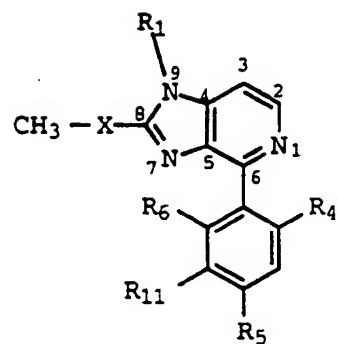
TABLE 3



(A)



(B)



(C)

| Ex. No. | X | R ⁴ | R ⁵ | R ¹¹ | R ⁶ | R ¹ | mp, °C |
|---------|-----------------|----------------|-----------------|-----------------|----------------|--|-----------|
| 3001 | CH ₂ | Cl | Cl | H | H | C(=O)OC ₂ H ₅ | - |
| 3002 | CH ₂ | Cl | Cl | H | H | C(=O)OC ₃ H ₇ | 90-91 |
| 3003 | CH ₂ | Cl | Cl | H | H | C(=O)OC ₄ H ₉ | 57-59 |
| 3004 | CH ₂ | Cl | Cl | H | H | C(=O)OCH(CH ₃) ₂ | 80-81 |
| 3005 | CH ₂ | Cl | Cl | H | H | C(=O)OCH ₂ CH(CH ₃) ₂ | 60-62 |
| 3006 | CH ₂ | Cl | Cl | H | H | C(=O)N(CH ₃) ₂ | - |
| 3007 | CH ₂ | Cl | Cl | H | H | C(=O)N(C ₂ H ₅) ₂ | 120-123 |
| 3008 | CH ₂ | Cl | Cl | H | H | C(=O)N[CH(CH ₃) ₂] ₂ | 147-149 |
| 3009 | CH ₂ | Cl | Cl | H | H | C(=O)(1-morpholinyl) | 158-159 |
| 3010 | CH ₂ | Cl | Cl | H | H | SO ₂ C ₆ H ₅ | 132-133 |
| 3011 | CH ₂ | Cl | Cl | H | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | 154-155 |
| 3012 | CH ₂ | Cl | Cl | H | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | 156-158 |
| 3013 | CH ₂ | Cl | Cl | H | H | SO ₂ -(2-thienyl) | 176-178 |
| 3014 | CH ₂ | Cl | Cl | H | H | SO ₂ CH ₂ C ₆ H ₅ | 127-129 |
| 3015 | CH ₂ | Cl | Cl | H | H | SO ₂ C ₃ H ₇ | 100-101 |
| 3016 | CH ₂ | Cl | Cl | H | H | SO ₂ C ₄ H ₉ | 79-80 |
| 3017 | CH ₂ | Cl | Cl | H | H | C(=O)-(2-Cl-C ₆ H ₄) | 110-113 |
| 3018 | CH ₂ | Cl | CF ₃ | H | H | C(=O)OC ₂ H ₅ | - |
| 3019 | CH ₂ | Cl | CF ₃ | H | H | C(=O)OC ₃ H ₇ | - |

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| 3020 | CH ₂ | Cl | CF ₃ | H | H | C(=O)OC ₄ H ₉ | - |
| 3021 | CH ₂ | Cl | CF ₃ | H | H | C(=O)OCH(CH ₃) ₂ | - |
| 3022 | CH ₂ | Cl | CF ₃ | H | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3023 | CH ₂ | Cl | CF ₃ | H | H | C(=O)N(CH ₃) ₂ | - |
| 3024 | CH ₂ | Cl | CF ₃ | H | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3025 | CH ₂ | Cl | CF ₃ | H | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3026 | CH ₂ | Cl | CF ₃ | H | H | C(=O)(1-morpholinyl) | - |
| 3027 | CH ₂ | Cl | CF ₃ | H | H | SO ₂ C ₆ H ₅ | - |
| 3028 | CH ₂ | Cl | CF ₃ | H | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3029 | CH ₂ | Cl | CF ₃ | H | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3030 | CH ₂ | Cl | CF ₃ | H | H | SO ₂ -(2-thienyl) | - |
| 3031 | CH ₂ | Cl | CF ₃ | H | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3032 | CH ₂ | Cl | CF ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3033 | CH ₂ | Cl | CF ₃ | H | H | SO ₂ C ₄ H ₉ | - |
| 3034 | CH ₂ | Cl | CF ₃ | H | H | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3035 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)OC ₂ H ₅ | - |
| 3036 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)OC ₃ H ₇ | - |
| 3037 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)OC ₄ H ₉ | - |
| 3038 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)OCH(CH ₃) ₂ | - |
| 3039 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3040 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)N(CH ₃) ₂ | - |
| 3041 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3042 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3043 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)(1-morpholinyl) | - |
| 3044 | CH ₂ | Cl | OCH ₃ | H | H | SO ₂ C ₆ H ₅ | - |
| 3045 | CH ₂ | Cl | OCH ₃ | H | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3046 | CH ₂ | Cl | OCH ₃ | H | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3047 | CH ₂ | Cl | OCH ₃ | H | H | SO ₂ -(2-thienyl) | - |
| 3048 | CH ₂ | Cl | OCH ₃ | H | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3049 | CH ₂ | Cl | OCH ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3050 | CH ₂ | Cl | OCH ₃ | H | H | SO ₂ C ₄ H ₉ | - |
| 3051 | CH ₂ | Cl | OCH ₃ | H | H | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3052 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)OC ₂ H ₅ | - |
| 3053 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)OC ₃ H ₇ | - |
| 3054 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)OC ₄ H ₉ | - |
| 3055 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)OCH(CH ₃) ₂ | - |
| 3056 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3057 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)N(CH ₃) ₂ | - |

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|------|-----------------|-----------------|------------------|---|---|--|---|
| 3058 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3059 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3060 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)(1-morpholinyl) | - |
| 3061 | CH ₂ | Cl | OCF ₃ | H | H | SO ₂ C ₆ H ₅ | - |
| 3062 | CH ₂ | Cl | OCF ₃ | H | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3063 | CH ₂ | Cl | OCF ₃ | H | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3064 | CH ₂ | Cl | OCF ₃ | H | H | SO ₂ -(2-thienyl) | - |
| 3065 | CH ₂ | Cl | OCF ₃ | H | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3066 | CH ₂ | Cl | OCF ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3067 | CH ₂ | Cl | OCF ₃ | H | H | SO ₂ C ₄ H ₉ | - |
| 3068 | CH ₂ | Cl | OCF ₃ | H | H | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3069 | CH ₂ | Cl | CH ₃ | H | H | C(=O)OC ₂ H ₅ | - |
| 3070 | CH ₂ | Cl | CH ₃ | H | H | C(=O)OC ₃ H ₇ | - |
| 3071 | CH ₂ | Cl | CH ₃ | H | H | C(=O)OC ₄ H ₉ | - |
| 3072 | CH ₂ | Cl | CH ₃ | H | H | C(=O)OCH(CH ₃) ₂ | - |
| 3073 | CH ₂ | Cl | CH ₃ | H | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3074 | CH ₂ | Cl | CH ₃ | H | H | C(=O)N(CH ₃) ₂ | - |
| 3075 | CH ₂ | Cl | CH ₃ | H | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3076 | CH ₂ | Cl | CH ₃ | H | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3077 | CH ₂ | Cl | CH ₃ | H | H | C(=O)(1-morpholinyl) | - |
| 3078 | CH ₂ | Cl | CH ₃ | H | H | SO ₂ C ₆ H ₅ | - |
| 3079 | CH ₂ | Cl | CH ₃ | H | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3080 | CH ₂ | Cl | CH ₃ | H | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3081 | CH ₂ | Cl | CH ₃ | H | H | SO ₂ -(2-thienyl) | - |
| 3082 | CH ₂ | Cl | CH ₃ | H | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3083 | CH ₂ | Cl | CH ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3084 | CH ₂ | Cl | CH ₃ | H | H | SO ₂ C ₄ H ₉ | - |
| 3085 | CH ₂ | Cl | CH ₃ | H | H | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3086 | CH ₂ | CF ₃ | Cl | H | H | C(=O)OC ₂ H ₅ | - |
| 3087 | CH ₂ | CF ₃ | Cl | H | H | C(=O)OC ₃ H ₇ | - |
| 3088 | CH ₂ | CF ₃ | Cl | H | H | C(=O)OC ₄ H ₉ | - |
| 3089 | CH ₂ | CF ₃ | Cl | H | H | C(=O)OCH(CH ₃) ₂ | - |
| 3090 | CH ₂ | CF ₃ | Cl | H | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3091 | CH ₂ | CF ₃ | Cl | H | H | C(=O)N(CH ₃) ₂ | - |
| 3092 | CH ₂ | CF ₃ | Cl | H | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3093 | CH ₂ | CF ₃ | Cl | H | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3094 | CH ₂ | CF ₃ | Cl | H | H | C(=O)(1-morpholinyl) | - |
| 3095 | CH ₂ | CF ₃ | Cl | H | H | SO ₂ C ₆ H ₅ | - |

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|------|-----------------|-----------------|------------------|---|---|--|---|
| 3096 | CH ₂ | CF ₃ | Cl | H | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3097 | CH ₂ | CF ₃ | Cl | H | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3098 | CH ₂ | CF ₃ | Cl | H | H | SO ₂ -(2-thienyl) | - |
| 3099 | CH ₂ | CF ₃ | Cl | H | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3100 | CH ₂ | CF ₃ | Cl | H | H | SO ₂ C ₃ H ₇ | - |
| 3101 | CH ₂ | CF ₃ | Cl | H | H | SO ₂ C ₄ H ₉ | - |
| 3102 | CH ₂ | CF ₃ | Cl | H | H | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3103 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)OC ₂ H ₅ | - |
| 3104 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)OC ₃ H ₇ | - |
| 3105 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)OC ₄ H ₉ | - |
| 3106 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)OCH(CH ₃) ₂ | - |
| 3107 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3108 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)N(CH ₃) ₂ | - |
| 3109 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3110 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3111 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)(1-morpholinyl) | - |
| 3112 | CH ₂ | CF ₃ | OCH ₃ | H | H | SO ₂ C ₆ H ₅ | - |
| 3113 | CH ₂ | CF ₃ | OCH ₃ | H | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3114 | CH ₂ | CF ₃ | OCH ₃ | H | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3115 | CH ₂ | CF ₃ | OCH ₃ | H | H | SO ₂ -(2-thienyl) | - |
| 3116 | CH ₂ | CF ₃ | OCH ₃ | H | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3117 | CH ₂ | CF ₃ | OCH ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3118 | CH ₂ | CF ₃ | OCH ₃ | H | H | SO ₂ C ₄ H ₉ | - |
| 3119 | CH ₂ | CF ₃ | OCH ₃ | H | H | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3120 | CH ₂ | CF ₃ | F | H | H | C(=O)OC ₂ H ₅ | - |
| 3121 | CH ₂ | CF ₃ | F | H | H | C(=O)OC ₃ H ₇ | - |
| 3122 | CH ₂ | CF ₃ | F | H | H | C(=O)OC ₄ H ₉ | - |
| 3123 | CH ₂ | CF ₃ | F | H | H | C(=O)OCH(CH ₃) ₂ | - |
| 3124 | CH ₂ | CF ₃ | F | H | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3125 | CH ₂ | CF ₃ | F | H | H | C(=O)N(CH ₃) ₂ | - |
| 3126 | CH ₂ | CF ₃ | F | H | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3127 | CH ₂ | CF ₃ | F | H | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3128 | CH ₂ | CF ₃ | F | H | H | C(=O)(1-morpholinyl) | - |
| 3129 | CH ₂ | CF ₃ | F | H | H | SO ₂ C ₆ H ₅ | - |
| 3130 | CH ₂ | CF ₃ | F | H | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3131 | CH ₂ | CF ₃ | F | H | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3132 | CH ₂ | CF ₃ | F | H | H | SO ₂ -(2-thienyl) | - |
| 3133 | CH ₂ | CF ₃ | F | H | H | SO ₂ CH ₂ C ₆ H ₅ | - |

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|------|-----------------|-----------------|------------------|-----------------|---|--|---|
| 3134 | CH ₂ | CF ₃ | F | H | H | SO ₂ C ₃ H ₇ | - |
| 3135 | CH ₂ | CF ₃ | F | H | H | SO ₂ C ₄ H ₉ | - |
| 3136 | CH ₂ | CF ₃ | F | H | H | C(=O) - (2-Cl-C ₆ H ₄) | - |
| 3137 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O)OC ₂ H ₅ | - |
| 3138 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O)OC ₃ H ₇ | - |
| 3139 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O)OC ₄ H ₉ | - |
| 3140 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O)OCH(CH ₃) ₂ | - |
| 3141 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3142 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O)N(CH ₃) ₂ | - |
| 3143 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3144 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3145 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O)(1-morpholinyl) | - |
| 3146 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | SO ₂ C ₆ H ₅ | - |
| 3147 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3148 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3149 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | SO ₂ -(2-thienyl) | - |
| 3150 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3151 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | SO ₂ C ₃ H ₇ | - |
| 3152 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | SO ₂ C ₄ H ₉ | - |
| 3153 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C(=O) - (2-Cl-C ₆ H ₄) | - |
| 3154 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O)OC ₂ H ₅ | - |
| 3155 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O)OC ₃ H ₇ | - |
| 3156 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O)OC ₄ H ₉ | - |
| 3157 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O)OCH(CH ₃) ₂ | - |
| 3158 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3159 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O)N(CH ₃) ₂ | - |
| 3160 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3161 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3162 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O)(1-morpholinyl) | - |
| 3163 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | SO ₂ C ₆ H ₅ | - |
| 3164 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3165 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3166 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | SO ₂ -(2-thienyl) | - |
| 3167 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3168 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | SO ₂ C ₃ H ₇ | - |
| 3169 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | SO ₂ C ₄ H ₉ | - |
| 3170 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C(=O) - (2-Cl-C ₆ H ₄) | - |
| 3171 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)OC ₂ H ₅ | - |

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|------|-----------------|-----------------|------------------|---|-----------------|--|---|
| 3172 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)OC ₃ H ₇ | - |
| 3173 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)OC ₄ H ₉ | - |
| 3174 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)OCH(CH ₃) ₂ | - |
| 3175 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3176 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)N(CH ₃) ₂ | - |
| 3177 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3178 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3179 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)(1-morpholinyl) | - |
| 3180 | CH ₂ | CH ₃ | OCH ₃ | F | H | SO ₂ C ₆ H ₅ | - |
| 3181 | CH ₂ | CH ₃ | OCH ₃ | F | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3182 | CH ₂ | CH ₃ | OCH ₃ | F | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3183 | CH ₂ | CH ₃ | OCH ₃ | F | H | SO ₂ -(2-thienyl) | - |
| 3184 | CH ₂ | CH ₃ | OCH ₃ | F | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3185 | CH ₂ | CH ₃ | OCH ₃ | F | H | SO ₂ C ₃ H ₇ | - |
| 3186 | CH ₂ | CH ₃ | OCH ₃ | F | H | SO ₂ C ₄ H ₉ | - |
| 3187 | CH ₂ | CH ₃ | OCH ₃ | F | H | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3188 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)OC ₂ H ₅ | - |
| 3189 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)OC ₃ H ₇ | - |
| 3190 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)OC ₄ H ₉ | - |
| 3191 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)OCH(CH ₃) ₂ | - |
| 3192 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3193 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)N(CH ₃) ₂ | - |
| 3194 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)N(C ₂ H ₅) ₂ | - |
| 3195 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3196 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)(1-morpholinyl) | - |
| 3197 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | SO ₂ C ₆ H ₅ | - |
| 3198 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3199 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3200 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | SO ₂ -(2-thienyl) | - |
| 3201 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3202 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | SO ₂ C ₃ H ₇ | - |
| 3203 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | SO ₂ C ₄ H ₉ | - |
| 3204 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3205 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)OC ₂ H ₅ | - |
| 3206 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)OC ₃ H ₇ | - |
| 3207 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)OC ₄ H ₉ | - |
| 3208 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)OCH(CH ₃) ₂ | - |
| 3209 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)OCH ₂ CH(CH ₃) ₂ | - |

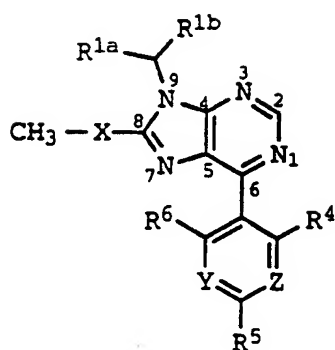
| | | | | | | | |
|------|-----------------|-----------------|------------------|------------------|-----------------|--|---|
| 3210 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)N(CH ₃) ₂ | - |
| 3211 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)N(C ₂ H ₅) ₂ | - |
| 3212 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3213 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)(1-morpholinyl) | - |
| 3214 | CH ₂ | Cl | Cl | H | CH ₃ | SO ₂ C ₆ H ₅ | - |
| 3215 | CH ₂ | Cl | Cl | H | CH ₃ | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3216 | CH ₂ | Cl | Cl | H | CH ₃ | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3217 | CH ₂ | Cl | Cl | H | CH ₃ | SO ₂ -(2-thienyl) | - |
| 3218 | CH ₂ | Cl | Cl | H | CH ₃ | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3219 | CH ₂ | Cl | Cl | H | CH ₃ | SO ₂ C ₃ H ₇ | - |
| 3220 | CH ₂ | Cl | Cl | H | CH ₃ | SO ₂ C ₄ H ₉ | - |
| 3221 | CH ₂ | Cl | Cl | H | CH ₃ | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3222 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)OC ₂ H ₅ | - |
| 3223 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)OC ₃ H ₇ | - |
| 3224 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)OC ₄ H ₉ | - |
| 3225 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)OCH(CH ₃) ₂ | - |
| 3226 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)OCH ₂ CH(CH ₃) ₂ | - |
| 3227 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)N(CH ₃) ₂ | - |
| 3228 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)N(C ₂ H ₅) ₂ | - |
| 3229 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)N[CH(CH ₃) ₂] ₂ | - |
| 3230 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)(1-morpholinyl) | - |
| 3231 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | SO ₂ C ₆ H ₅ | - |
| 3232 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | SO ₂ (4-CH ₃ -C ₆ H ₄) | - |
| 3233 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | SO ₂ (4-OCH ₃ -C ₆ H ₄) | - |
| 3234 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | SO ₂ -(2-thienyl) | - |
| 3235 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | SO ₂ CH ₂ C ₆ H ₅ | - |
| 3236 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | SO ₂ C ₃ H ₇ | - |
| 3237 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | SO ₂ C ₄ H ₉ | - |
| 3238 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C(=O)-(2-Cl-C ₆ H ₄) | - |
| 3239 | O | Cl | Cl | H | H | SO ₂ C ₃ H ₇ | - |
| 3240 | O | Cl | CF ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3241 | O | Cl | OCH ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3242 | O | Cl | OCF ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3243 | O | Cl | CH ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3244 | O | CF ₃ | Cl | H | H | SO ₂ C ₃ H ₇ | - |
| 3245 | O | CF ₃ | OCH ₃ | H | H | SO ₂ C ₃ H ₇ | - |
| 3246 | O | CH ₃ | OCH ₃ | CH ₃ | H | SO ₂ C ₃ H ₇ | - |
| 3247 | O | CH ₃ | OCH ₃ | Cl | H | SO ₂ C ₃ H ₇ | - |

| | | | | | | | |
|------|-----------------|-----------------|------------------|---|-----------------|---|---------|
| 3248 | O | CH ₃ | OCH ₃ | F | H | SO ₂ C ₃ H ₇ | - |
| 3249 | O | CH ₃ | CH ₃ | H | CH ₃ | SO ₂ C ₃ H ₇ | - |
| 3250 | O | Cl | Cl | H | CH ₃ | SO ₂ C ₃ H ₇ | - |
| 3251 | CH ₂ | Cl | Cl | H | H | C(=O) - (3-Cl-C ₆ H ₄) | 115-118 |

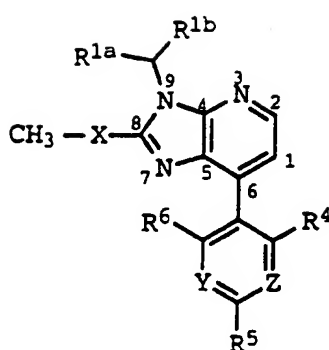
5 The methods used in the preparation of the compounds of
 Structure A of Table 1 may be used for the compounds of
 Structure A of Table 4. For example, replacing variously-
 substituted pyridine- and pyrimidineboronic acids for
 benzeneboronic acids in the palladium-catalyzed aryl cross-
 coupling method (see Examples 35 or 831) will afford the
 10 desired 6-pyridyl- or 6-pyrimidylpurine compounds.

15 The methods of Schemes 13 and 14 may be used to
 prepare many of the examples of Structure B and Structure C
 contained in Table 4, with minor procedural modifications
 where necessary and use of reagents of the appropriate
 structure.

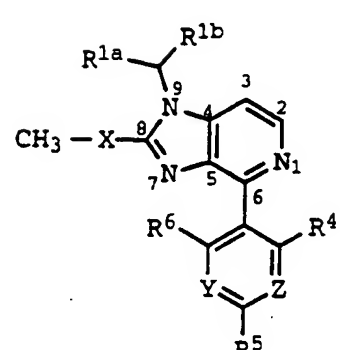
TABLE 4



(A)



(B)



(C)

5

| Ex. No. | X | R ⁴ | Z | R ⁵ | Y | R ⁶ | R ^{1a} | R ^{1b} | m.p., °C |
|---------|-----------------|-----------------|----|----------------------------------|---|-----------------|---------------------------------|---|-------------|
| 4001 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4002 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | CH ₃ | c-C ₃ H ₅ | - |
| 4003 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4004 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4005 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4006 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | CH ₃ | C ₃ H ₇ | - |
| 4007 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4008 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4009 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4010 | CH ₂ | CH ₃ | CH | N(CH ₃) ₂ | N | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4011 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4012 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | CH ₃ | c-C ₃ H ₅ | - |
| 4013 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4014 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4015 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4016 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | CH ₃ | C ₃ H ₇ | - |
| 4017 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4018 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4019 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4020 | O | CH ₃ | CH | N(CH ₃) ₂ | N | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4021 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4022 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | CH ₃ | c-C ₃ H ₅ | - |

| | | | | | | | | | |
|------|-----------------|-----------------|----|------------------|---|-----------------|---------------------------------|---|---|
| 4023 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4024 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4025 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4026 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 4027 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 4028 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 4029 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 4030 | CH ₂ | CH ₃ | CH | CH ₃ | N | CH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4031 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4032 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 4033 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4034 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4035 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4036 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 4037 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 4038 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 4039 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 4040 | O | CH ₃ | CH | CH ₃ | N | CH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4041 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4042 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | CH ₃ | c-C ₃ H ₅ | - |
| 4043 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4044 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4045 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4046 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | CH ₃ | C ₃ H ₇ | - |
| 4047 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4048 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4049 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4050 | CH ₂ | CH ₃ | CH | SCH ₃ | N | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4051 | O | CH ₃ | CH | SCH ₃ | N | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4052 | O | CH ₃ | CH | SCH ₃ | N | H | CH ₃ | c-C ₃ H ₅ | - |
| 4053 | O | CH ₃ | CH | SCH ₃ | N | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4054 | O | CH ₃ | CH | SCH ₃ | N | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4055 | O | CH ₃ | CH | SCH ₃ | N | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4056 | O | CH ₃ | CH | SCH ₃ | N | H | CH ₃ | C ₃ H ₇ | - |
| 4057 | O | CH ₃ | CH | SCH ₃ | N | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4058 | O | CH ₃ | CH | SCH ₃ | N | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4059 | O | CH ₃ | CH | SCH ₃ | N | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4060 | O | CH ₃ | CH | SCH ₃ | N | H | H | 4-CH ₃ O-C ₆ H ₄ | - |

| | | | | | | | | | |
|------|-----------------|------------------|---|-----------------|---|------------------|---------------------------------|---|---|
| 4061 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4062 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 4063 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4064 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4065 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4066 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 4067 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 4068 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 4069 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 4070 | CH ₂ | SCH ₃ | N | CH ₃ | N | SCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4071 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4072 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 4073 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4074 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4075 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4076 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 4077 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 4078 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 4079 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 4080 | O | SCH ₃ | N | CH ₃ | N | SCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4081 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4082 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 4083 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4084 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4085 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4086 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 4087 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 4088 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 4089 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 4090 | CH ₂ | CH ₃ | N | CH ₃ | N | CH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4091 | O | CH ₃ | N | CH ₃ | N | CH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4092 | O | CH ₃ | N | CH ₃ | N | CH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 4093 | O | CH ₃ | N | CH ₃ | N | CH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4094 | O | CH ₃ | N | CH ₃ | N | CH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4095 | O | CH ₃ | N | CH ₃ | N | CH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4096 | O | CH ₃ | N | CH ₃ | N | CH ₃ | CH ₃ | C ₃ H ₇ | - |
| 4097 | O | CH ₃ | N | CH ₃ | N | CH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 4098 | O | CH ₃ | N | CH ₃ | N | CH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |

| | | | | | | | | | |
|------|-----------------|-----------------|----|----------------------------------|----|-----------------|---------------------------------|---|---|
| 4099 | O | CH ₃ | N | CH ₃ | N | CH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 4100 | O | CH ₃ | N | CH ₃ | N | CH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4101 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4102 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | CH ₃ | c-C ₃ H ₅ | - |
| 4103 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4104 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4105 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4106 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | CH ₃ | C ₃ H ₇ | - |
| 4107 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4108 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4109 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4110 | CH ₂ | CH ₃ | CH | CH ₃ | N | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4111 | O | CH ₃ | CH | CH ₃ | N | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4112 | O | CH ₃ | CH | CH ₃ | N | H | CH ₃ | c-C ₃ H ₅ | - |
| 4113 | O | CH ₃ | CH | CH ₃ | N | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4114 | O | CH ₃ | CH | CH ₃ | N | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4115 | O | CH ₃ | CH | CH ₃ | N | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4116 | O | CH ₃ | CH | CH ₃ | N | H | CH ₃ | C ₃ H ₇ | - |
| 4117 | O | CH ₃ | CH | CH ₃ | N | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4118 | O | CH ₃ | CH | CH ₃ | N | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4119 | O | CH ₃ | CH | CH ₃ | N | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4120 | O | CH ₃ | CH | CH ₃ | N | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4121 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4122 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | CH ₃ | c-C ₃ H ₅ | - |
| 4123 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4124 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4125 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4126 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | CH ₃ | C ₃ H ₇ | - |
| 4127 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4128 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4129 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4130 | CH ₂ | CH ₃ | N | N(CH ₃) ₂ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4131 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4132 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | CH ₃ | c-C ₃ H ₅ | - |
| 4133 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4134 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4135 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4136 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | CH ₃ | C ₃ H ₇ | - |

| | | | | | | | | | |
|------|-----------------|------------------|---|----------------------------------|----|---|---------------------------------|---|---------|
| 4137 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4138 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4139 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4140 | O | CH ₃ | N | N(CH ₃) ₂ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4141 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4142 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | CH ₃ | c-C ₃ H ₅ | - |
| 4143 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4144 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4145 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4146 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | CH ₃ | C ₃ H ₇ | - |
| 4147 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4148 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4149 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4150 | CH ₂ | CH ₃ | N | CH ₃ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4151 | O | CH ₃ | N | CH ₃ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4152 | O | CH ₃ | N | CH ₃ | CH | H | CH ₃ | c-C ₃ H ₅ | - |
| 4153 | O | CH ₃ | N | CH ₃ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4154 | O | CH ₃ | N | CH ₃ | CH | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4155 | O | CH ₃ | N | CH ₃ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4156 | O | CH ₃ | N | CH ₃ | CH | H | CH ₃ | C ₃ H ₇ | - |
| 4157 | O | CH ₃ | N | CH ₃ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4158 | O | CH ₃ | N | CH ₃ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4159 | O | CH ₃ | N | CH ₃ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4160 | O | CH ₃ | N | CH ₃ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4161 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | 120-121 |
| 4162 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | CH ₃ | c-C ₃ H ₅ | - |
| 4163 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4164 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₃ H ₇ | c-C ₃ H ₇ | - |
| 4165 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4166 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | CH ₃ | C ₃ H ₇ | oil |
| 4167 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4168 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4169 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4170 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4171 | O | OCH ₃ | N | OCH ₃ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | oil |
| 4172 | O | OCH ₃ | N | OCH ₃ | CH | H | CH ₃ | c-C ₃ H ₅ | - |
| 4173 | O | OCH ₃ | N | OCH ₃ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4174 | O | OCH ₃ | N | OCH ₃ | CH | H | C ₃ H ₇ | c-C ₃ H ₅ | - |

| | | | | | | | | | |
|------|-----------------|----------------------------------|---|----------------------------------|----|---|---------------------------------|---|---|
| 4175 | O | OCH ₃ | N | OCH ₃ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4176 | O | OCH ₃ | N | OCH ₃ | CH | H | CH ₃ | C ₃ H ₇ | - |
| 4177 | O | OCH ₃ | N | OCH ₃ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4178 | O | OCH ₃ | N | OCH ₃ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4179 | O | OCH ₃ | N | OCH ₃ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4180 | O | OCH ₃ | N | OCH ₃ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4181 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4182 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | CH ₃ | c-C ₃ H ₅ | - |
| 4183 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4184 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4185 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4186 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | CH ₃ | C ₃ H ₇ | - |
| 4187 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4188 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4189 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4190 | CH ₂ | OCH ₃ | N | N(CH ₃) ₂ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4191 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4192 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | CH ₃ | c-C ₃ H ₅ | - |
| 4193 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4194 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4195 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4196 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | CH ₃ | C ₃ H ₇ | - |
| 4197 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4198 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4199 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4200 | O | OCH ₃ | N | N(CH ₃) ₂ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4201 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4202 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | CH ₃ | c-C ₃ H ₅ | - |
| 4203 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4204 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4205 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4206 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | CH ₃ | C ₃ H ₇ | - |
| 4207 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4208 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4209 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4210 | CH ₂ | N(CH ₃) ₂ | N | OCH ₃ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4211 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 4212 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | CH ₃ | c-C ₃ H ₅ | - |

| | | | | | | | | | |
|------|-----------------|----------------------------------|---|------------------|----|---|---------------------------------|---|---|
| 4213 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 4214 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 4215 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 4216 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | CH ₃ | C ₃ H ₇ | - |
| 4217 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₂ H ₅ | C ₃ H ₇ | - |
| 4218 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₃ H ₇ | C ₃ H ₇ | - |
| 4219 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | C ₂ H ₅ | C ₄ H ₉ | - |
| 4220 | O | N(CH ₃) ₂ | N | OCH ₃ | CH | H | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 4221 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₂ H ₅ | 2-furanyl | - |
| 4222 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₃ H ₇ | 2-furanyl | - |
| 4223 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₂ H ₅ | b | - |
| 4224 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₃ H ₇ | b | - |
| 4225 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₆ H ₅ | b | - |
| 4226 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | c-C ₃ H ₅ | b | - |
| 4227 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | CH ₃ | CH=CHCH ₃ | - |
| 4228 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | C ₃ H ₇ | CH=CH ₂ | - |
| 4229 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | CH ₃ | C ₆ H ₅ | - |
| 4230 | CH ₂ | OCH ₃ | N | OCH ₃ | CH | H | CH ₃ | c-C ₄ H ₇ | - |

Key:

5 a) Where the compound is indicated as an "oil", spectral data is provided below:

Example 4166 elemental analysis: calc. for C₁₉H₂₅N₅O₂ C 64.20, H 7.10, N 19.70; observed C 64.13, H 6.67, N 19.30.

Example 4171 elemental analysis: calc. for C₂₀H₂₃N₅O₃ C 62.98, H 6.09, N 18.36; observed C 62.80, H 6.10, N 18.19.

10 b) C=C-CH₃

15 The methods used in the preparation of the compounds of Table 1 may be employed in the synthesis of those compounds of Structure A in Table 5 and Table 5A. The methods employed to make the analogues bearing a benzofuran group are illustrated in the following examples.

20 The methods of Schemes 13 and 14 may be used to prepare many of the examples of Structure B and Structure C

contained in Table 5 and Table 5A, with minor procedural modifications where necessary and use of reagents of the appropriate structure.

5

Example 5001

Preparation of 9-Dicyclopropylmethyl-8-ethyl-6-(6-methyl-2,3-dihydrobenzofuran-5-yl)purine

- 10 Part A. Sodium hydride dispersion in mineral oil (5.05 g, 50% w/w, 105 mmol) was washed with hexane and dried under vacuum. DMF (100 mL) was added, the slurry was cooled to 0 °C, and treated with a solution of *m*-cresol (10 mL, 95.6 mmol) in DMF (20 mL). The resulting mixture was allowed to stir for 1 h,
- 15 then was treated with chloromethyl methyl ether (8.00 mL, 105 mmol) by syringe. The mixture was stirred overnight, then poured into ethyl acetate (200 mL). This was washed with water (3 x 200 mL) and brine (100 mL), and the aqueous phases were back-extracted in sequence with ethyl acetate. The extracts
- 20 were combined, dried over magnesium sulfate, filtered and evaporated. The oily product was purified by elution through a plug of silica gel with 10:90 ethyl acetate-hexane. Evaporation then afforded the pure product, 3-(methoxymethoxy)toluene, as an oil (13.93 g, 91.5 mmol, 96%).
- 25 TLC R_f 0.46 (10:90 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): d 7.17 (1H, t, $J = 7.7$ Hz), 6.86-6.81 (3H, m), 5.17 (2H, s), 3.48 (3H, s), 2.33 (3H, s). MS (H_2O -GC/MS): m/e 153 (60), 121 (100).

30

- Part B. A solution of 3-(methoxymethoxy)toluene (5.00 g, 32.9 mmol) and TMEDA (5.30 mL, 35.1 mmol) in THF (50 mL) was cooled to 0 °C, and treated with a hexane solution of *n*-butyllithium (22.0 mL, 1.6 M, 35.2 mmol). After 4 hours, the solution was
- 35 cooled to -78 °C, and treated dropwise with ethylene oxide (2.00 mL, 40 mmol, condensed from a lecture bottle through a cold-finger into a graduated dropping funnel). The mixture was allowed to stir and warm to ambient temperature overnight,

then was poured into satd. aq. ammonium chloride solution (120 mL). This was extracted with ethyl acetate (2 x 120 mL), and the extracts were washed in sequence with brine, combined, dried over magnesium sulfate, filtered and evaporated. The residual oil was separated by column chromatography (10:90 ethyl acetate-hexane) to afford the desired product, 2-[2-(methoxymethoxy)-4-methylphenyl]ethanol, as a viscous liquid (2.25 g, 11.5 mmol, 35%), along with 2.50 g recovered starting material. The ¹H NMR spectrum showed regioselectivity in excess of 10:1. TLC R_f 0.09 (10:90 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 7.06 (1H, d, J = 7.7 Hz), 6.92 (1H, br s), 6.78 (1H, br d, J = 7.7 Hz), 5.20 (2H, s), 3.83 (2H, q, J = 6.4 Hz), 3.49 (3H, s), 2.89 (2H, t, J = 6.6 Hz), 2.32 (3H, s), 1.61 (1H, t, J = 5.9 Hz). MS (NH₃-DCI): m/e 214 (76), 212 (100), 197 (9), 182 (30), 165 (38).

Part C. A solution of the MOM compound from Part B (1.84 g, 9.38 mmol) was dissolved in 1:1 THF-isopropanol (20 mL), and treated with HCl in dioxane (2.5 mL, 4 N, 10.0 mmol). The reaction was stirred at ambient temperature overnight. Aqueous workup gave sufficiently pure product, 2-(2-hydroxy-4-methylphenyl)ethanol.

Part D. A solution of the diol from Part C (ca. 9 mmol) and triphenylphosphine (2.83 g, 10.8 mmol) in THF (20 mL) was cooled to 0 °C, and treated with diethyl azodicarboxylate (1.70 mL, 10.8 mmol) by syringe. The solution was stirred overnight, then evaporated, and the residue separated by a flash column to afford the product, 6-methyl-2,3-dihydrobenzofuran (780 mg, 5.81 mmol, 65%). TLC R_f 0.29 (2:98 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 7.07 (1H, d, J = 7.4 Hz), 6.66 (1H, d, J = 7.4 Hz), 6.62 (1H, s), 4.54 (2H, t, J = 8.6 Hz), 3.16 (2H, t, J = 8.6 Hz), 2.30 (3H, s). MS (D₂O-GC/MS): m/e 135 (100).

Part E. A solution of the above compound (780 mg) and N-bromosuccinimide (1.24 g, 6.97 mmol) in dichloroethane (10 mL) was heated to reflux overnight, then cooled, filtered and

evaporated. Column chromatography (hexane, then 2:98 ethyl acetate-hexane) gave first 5-bromo-6-methylbenzofuran (270 mg, 1.27 mmol, 22%), then 5-bromo-6-methyl-2,3-dihydrobenzofuran (923 mg, 4.33 mol, 75%), both as solids. For the dihydro
5 product: TLC R_f 0.35 (2:98 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): d 7.31 (1H, s), 6.68 (1H, s), 4.56 (2H, t, J = 8.8 Hz), 3.17 (2H, t, J = 8.8 Hz), 2.33 (3H, s). MS (H_2O -GC/MS): m/e 215 (76), 213 (100).

10 Part F. A solution of the bromide from Part E (923 mg, 4.33 mmol) in tetrahydrofuran (20 mL) was cooled to -78°C , and treated with a hexane solution of *n*-butyllithium (3.0 mL, 1.6 M, 4.8 mmol). After 1 hour, the reaction mixture was treated with triisopropylborate (1.00 mL, 4.33 mmol) and allowed to
15 come to ambient temperature over 6 hrs. Then, 1 mL of 6 N aq. HCl and 3 mL water were added, and the resulting mixture was allowed to stir for 1 hr. It was poured into water (100 mL), and extracted with ethyl acetate (2 x 100 mL). The extracts were washed with brine (60 mL), combined, dried over sodium
20 sulfate, filtered and evaporated to afford a solid, which was purified by trituration with hexane to give 6-methyl-2,3-dihydrobenzofuran-5-boronic acid (718 mg, 4.03 mmol, 93%).

Part G. A mixture of the boronic acid from Part F (298 mg, 1.67 mmol), 6-chloro-9-dicyclopropylmethyl-8-ethylpurine (309
25 mg, 1.12 mmol), 2 N aqueous sodium carbonate solution (1.7 mL, 3.4 mmol) and triphenylphosphine (61 mg, 0.233 mmol) in DME (20 mL) was degassed by repeated cycles of brief vacuum pumping followed by nitrogen purging. To this was added
30 palladium (II) acetate (13 mg, 0.058 mmol), and the mixture was degassed again and then heated to reflux for 14 hours. It was cooled, and poured into water (100 mL). This mixture was extracted with ethyl acetate (2 x 100 mL), and the extracts were washed in sequence with brine (60 mL), combined, dried
35 over sodium sulfate, filtered and evaporated. The residual material was separated by column chromatography (silica gel, 20:80 ethyl acetate-hexane) to afford the title product as a solid. This was recrystallized to purity from ether (253 mg,

0.77 mmol, 69%). m.p. 147-148 °C. TLC R_f 0.18 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.88 (1H, s), 7.60 (1H, s), 6.77 (1H, s), 4.61 (2H, t, $J = 8.6$ Hz), 3.44 (1H, v br), 3.24 (2H, t, $J = 8.6$ Hz), 2.94 (2H, br), 2.44 (3H, s), 2.03 (2H, v br), 1.45 (3H, br t, $J = 6$ Hz), 0.89-0.79 (2H, m), 0.58 (2H, br), 0.50-0.40 (2H, m), 0.27-0.17 (2H, m). MS (NH_3 -CI): m/e 377 (4), 376 (27), 375 (100). Analysis calc'd for $\text{C}_{23}\text{H}_{26}\text{N}_4\text{O}$: C, 73.77; H, 7.01; N, 14.96; found: C, 73.69; H, 7.08; N, 14.40.

10

Examples 5201, 5231 and 5232

Preparation of 9-dicyclopropylmethyl-8-ethyl-6-(6-methylbenzofuran-5-yl)purine, 6-(2-bromo-6-methylbenzofuran-5-yl)-9-dicyclopropylmethyl-8-ethylpurine and 6-(7-bromo-6-methyl-2,3-dihydrobenzofuran-5-yl)-9-dicyclopropylmethyl-8-ethylpurine

A solution of the compound of Example 5001 (250 mg, 0.668 mmol) and N-bromosuccinimide (119 mg, 0.669 mmol) in 1,2-dichloroethane (10 mL) was heated to reflux for 12 hours, then cooled and evaporated. The resulting mixture was taken up in ether, filtered and evaporated, and the residual material was separated by flash chromatography (silica gel, 20:80 ethyl acetate-hexane) to afford, in order, the following three products:

6-(2-Bromo-6-methylbenzofuran-5-yl)-9-dicyclopropylmethyl-8-ethylpurine: m.p. 177-178 °C. TLC R_f 0.23 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.92 (1H, s), 7.85 (1H, s), 7.42 (1H, s), 6.74 (1H, s), 4.15 (1H, v br), 2.97 (2H, v br), 2.54 (3H, s), 2.00 (2H, v br), 1.44 (3H, br t, $J = 7$ Hz), 0.90-0.80 (2H, m), 0.63-0.53 (2H, m), 0.50-0.40 (2H, m), 0.26-0.16 (2H, m). MS (NH_3 -CI): m/e calc'd for $\text{C}_{23}\text{H}_{24}\text{BrN}_4\text{O}$: 451.1133, found 451.1132; 455 (3), 454 (25), 453 (99), 452 (31), 451 (100).

9-Dicyclopropylmethyl-8-ethyl-6-(6-methylbenzofuran-5-yl)purine: m.p. 139-141 °C. TLC R_f 0.16 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.92 (1H, s), 7.95 (1H, s), 7.60 (1H, d, $J = 2.2$ Hz), 7.48 (1H, d, $J = 0.7$ Hz), 6.78 (1H,

dd, $J = 2.2, 0.7$ Hz), 4.40 (1H, v br), 2.97 (2H, v br), 2.56 (3H, s), 2.04 (2H, v br), 1.44 (3H, br t, $J = 7$ Hz), 0.90-0.80 (2H, m), 0.62-0.52 (2H, m), 0.51-0.41 (2H, m), 0.29-0.18 (2H, m). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{23}\text{H}_{25}\text{N}_4\text{O}$: 373.2028, found

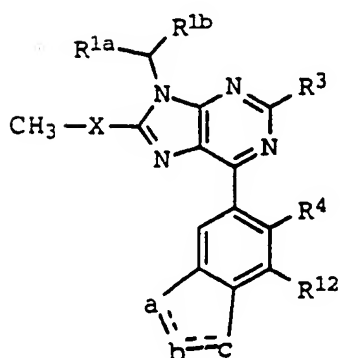
5 373.2033; 375 (3), 374 (26), 373 (100).

6-(7-Bromo-6-methyl-2,3-dihydrobenzofuran-5-yl)-9-

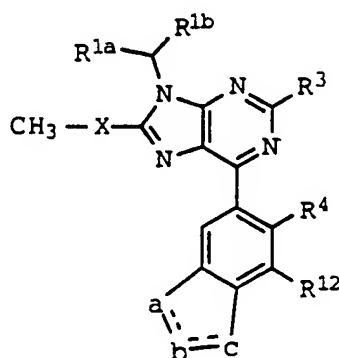
dicyclopropylmethyl-8-ethylpurine: m.p. 179-180 °C. TLC R_f 0.04 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.89 (1H, s), 7.47 (1H, s), 4.73 (2H, t, $J = 8.6$ Hz), 3.80 (1H, v br), 3.37 (2H, t, $J = 8.6$ Hz), 2.95 (2H, v br), 2.44 (3H, s), 1.44 (3H, br t, $J = 7$ Hz), 0.89-0.79 (2H, m), 0.61-0.52 (2H, m), 0.51-0.41 (2H, m), 0.28-0.18 (2H, m). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{23}\text{H}_{26}\text{BrN}_4\text{O}$: 453.1290, found 453.1285; 455 (98), 453 (100).

15

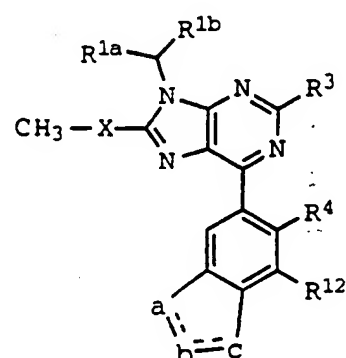
TABLE 5



(A)



(B)



(C)

20

| Ex. No. | X | R^3 | R^4 | a | b | c | R^{1a} | R^{1b} | m.p., °C |
|---------|---------------|-------|---------------|---------------|---------------|---|--------------------------|---|----------|
| 5001 | CH_2 | H | CH_3 | CH_2 | CH_2 | O | $\text{c-C}_3\text{H}_5$ | $\text{c-C}_3\text{H}_5$ | 147-148 |
| 5002 | CH_2 | H | CH_3 | CH_2 | CH_2 | O | H | 4-(CH_3O)- C_6H_4 | - |
| 5003 | CH_2 | H | CH_3 | CH_2 | CH_2 | O | CH_3 | $\text{c-C}_3\text{H}_5$ | - |
| 5004 | CH_2 | H | CH_3 | CH_2 | CH_2 | O | C_2H_5 | $\text{c-C}_3\text{H}_5$ | - |
| 5005 | CH_2 | H | CH_3 | CH_2 | CH_2 | O | C_3H_7 | $\text{c-C}_3\text{H}_5$ | - |

| | | | | | | | | | |
|------|-----------------|---|-----------------|-----------------|-----------------|-----------------|---------------------------------|---|---------|
| 5006 | CH ₂ | H | CH ₃ | CH ₂ | CH ₂ | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5007 | CH ₂ | H | CH ₃ | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5008 | CH ₂ | H | CH ₃ | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5009 | CH ₂ | H | CH ₃ | CH ₂ | CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5010 | CH ₂ | H | CH ₃ | CH ₂ | CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5011 | CH ₂ | H | CH ₃ | O | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | 168-169 |
| 5012 | CH ₂ | H | CH ₃ | O | CH ₂ | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5013 | CH ₂ | H | CH ₃ | O | CH ₂ | O | CH ₃ | c-C ₃ H ₅ | - |
| 5014 | CH ₂ | H | CH ₃ | O | CH ₂ | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5015 | CH ₂ | H | CH ₃ | O | CH ₂ | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5016 | CH ₂ | H | CH ₃ | O | CH ₂ | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5017 | CH ₂ | H | CH ₃ | O | CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5018 | CH ₂ | H | CH ₃ | O | CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5019 | CH ₂ | H | CH ₃ | O | CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5020 | CH ₂ | H | CH ₃ | O | CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5021 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5022 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5023 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | CH ₃ | c-C ₃ H ₅ | - |
| 5024 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5025 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5026 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5027 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | C ₂ H ₅ | C ₃ H ₇ | - |
| 5028 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | C ₂ H ₅ | C ₄ H ₉ | - |
| 5029 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | C ₃ H ₇ | C ₃ H ₇ | - |
| 5030 | CH ₂ | H | CH ₃ | O | CH ₂ | CH ₂ | CH ₃ | C ₃ H ₇ | - |
| 5031 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5032 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5033 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | CH ₃ | c-C ₃ H ₅ | - |
| 5034 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5035 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5036 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5037 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | C ₂ H ₅ | C ₃ H ₇ | - |
| 5038 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | C ₂ H ₅ | C ₄ H ₉ | - |
| 5039 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | C ₃ H ₇ | C ₃ H ₇ | - |
| 5040 | CH ₂ | H | CH ₃ | CH ₂ | O | CH ₂ | CH ₃ | C ₃ H ₇ | - |
| 5041 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5042 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5043 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | CH ₃ | c-C ₃ H ₅ | - |

| | | | | | | | | | |
|------|-----------------|---|-----------------|-----------------|-----------------|---|---------------------------------|---|---|
| 5044 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5045 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5046 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5047 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5048 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5049 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5050 | CH ₂ | H | Cl | CH ₂ | CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5051 | CH ₂ | H | Cl | O | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5052 | CH ₂ | H | Cl | O | CH ₂ | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5053 | CH ₂ | H | Cl | O | CH ₂ | O | CH ₃ | c-C ₃ H ₅ | - |
| 5054 | CH ₂ | H | Cl | O | CH ₂ | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5055 | CH ₂ | H | Cl | O | CH ₂ | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5056 | CH ₂ | H | Cl | O | CH ₂ | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5057 | CH ₂ | H | Cl | O | CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5058 | CH ₂ | H | Cl | O | CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5059 | CH ₂ | H | Cl | O | CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5060 | CH ₂ | H | Cl | O | CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5061 | O | H | CH ₃ | CH ₂ | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5062 | O | H | CH ₃ | CH ₂ | CH ₂ | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5063 | O | H | CH ₃ | CH ₂ | CH ₂ | O | CH ₃ | c-C ₃ H ₅ | - |
| 5064 | O | H | CH ₃ | CH ₂ | CH ₂ | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5065 | O | H | CH ₃ | CH ₂ | CH ₂ | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5066 | O | H | CH ₃ | CH ₂ | CH ₂ | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5067 | O | H | CH ₃ | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5068 | O | H | CH ₃ | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5069 | O | H | CH ₃ | CH ₂ | CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5070 | O | H | CH ₃ | CH ₂ | CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5071 | O | H | CH ₃ | O | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5072 | O | H | CH ₃ | O | CH ₂ | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5073 | O | H | CH ₃ | O | CH ₂ | O | CH ₃ | c-C ₃ H ₅ | - |
| 5074 | O | H | CH ₃ | O | CH ₂ | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5075 | O | H | CH ₃ | O | CH ₂ | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5076 | O | H | CH ₃ | O | CH ₂ | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5077 | O | H | CH ₃ | O | CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5078 | O | H | CH ₃ | O | CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5079 | O | H | CH ₃ | O | CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5080 | O | H | CH ₃ | O | CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5081 | O | H | Cl | CH ₂ | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |

| | | | | | | | | | |
|------|-----------------|-----------------|-----------------|-----------------|-----------------|----|-----------------------------------|---|---|
| 5082 | O | H | Cl | CH ₂ | CH ₂ | O | H | 4 - (CH ₃ O) - C ₆ H ₄ | - |
| 5083 | O | H | Cl | CH ₂ | CH ₂ | O | CH ₃ | c - C ₃ H ₅ | - |
| 5084 | O | H | Cl | CH ₂ | CH ₂ | O | C ₂ H ₅ | c - C ₃ H ₅ | - |
| 5085 | O | H | Cl | CH ₂ | CH ₂ | O | C ₃ H ₇ | c - C ₃ H ₅ | - |
| 5086 | O | H | Cl | CH ₂ | CH ₂ | O | C ₄ H ₉ | c - C ₃ H ₅ | - |
| 5087 | O | H | Cl | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5088 | O | H | Cl | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5089 | O | H | Cl | CH ₂ | CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5090 | O | H | Cl | CH ₂ | CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5091 | O | H | Cl | O | CH ₂ | O | c - C ₃ H ₅ | c - C ₃ H ₅ | - |
| 5092 | O | H | Cl | O | CH ₂ | O | H | 4 - (CH ₃ O) - C ₆ H ₄ | - |
| 5093 | O | H | Cl | O | CH ₂ | O | CH ₃ | c - C ₃ H ₅ | - |
| 5094 | O | H | Cl | O | CH ₂ | O | C ₂ H ₅ | c - C ₃ H ₅ | - |
| 5095 | O | H | Cl | O | CH ₂ | O | C ₃ H ₇ | c - C ₃ H ₅ | - |
| 5096 | O | H | Cl | O | CH ₂ | O | C ₄ H ₉ | c - C ₃ H ₅ | - |
| 5097 | O | H | Cl | O | CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5098 | O | H | Cl | O | CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5099 | O | H | Cl | O | CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5100 | O | H | Cl | O | CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5101 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | c - C ₃ H ₅ | c - C ₃ H ₅ | - |
| 5102 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | H | 4 - (CH ₃ O) - C ₆ H ₄ | - |
| 5103 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | CH ₃ | c - C ₃ H ₅ | - |
| 5104 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | C ₂ H ₅ | c - C ₃ H ₅ | - |
| 5105 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | C ₃ H ₇ | c - C ₃ H ₅ | - |
| 5106 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | C ₄ H ₉ | c - C ₃ H ₅ | - |
| 5107 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5108 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5109 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5110 | CH ₂ | CH ₃ | CH ₃ | CH ₂ | CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5111 | CH ₂ | H | Cl | O | C=O | NH | c - C ₃ H ₅ | c - C ₃ H ₅ | - |
| 5112 | CH ₂ | H | Cl | O | C=O | NH | H | 4 - (CH ₃ O) - C ₆ H ₄ | - |
| 5113 | CH ₂ | H | Cl | O | C=O | NH | CH ₃ | c - C ₃ H ₅ | - |
| 5114 | CH ₂ | H | Cl | O | C=O | NH | C ₂ H ₅ | c - C ₃ H ₅ | - |
| 5115 | CH ₂ | H | Cl | O | C=O | NH | C ₃ H ₇ | c - C ₃ H ₅ | - |
| 5116 | CH ₂ | H | Cl | O | C=O | NH | C ₄ H ₉ | c - C ₃ H ₅ | - |
| 5117 | CH ₂ | H | Cl | O | C=O | NH | C ₂ H ₅ | C ₃ H ₇ | - |
| 5118 | CH ₂ | H | Cl | O | C=O | NH | C ₂ H ₅ | C ₄ H ₉ | - |
| 5119 | CH ₂ | H | Cl | O | C=O | NH | C ₃ H ₇ | C ₃ H ₇ | - |

| | | | | | | | | | |
|------|-----------------|---|----|---|------------------|--------------------------------|---------------------------------|---|---|
| 5120 | CH ₂ | H | Cl | O | C=O | NH | CH ₃ | C ₃ H ₇ | - |
| 5121 | CH ₂ | H | Cl | O | C=O | NCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5122 | CH ₂ | H | Cl | O | C=O | NCH ₃ | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5123 | CH ₂ | H | Cl | O | C=O | NCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 5124 | CH ₂ | H | Cl | O | C=O | NCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5125 | CH ₂ | H | Cl | O | C=O | NCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5126 | CH ₂ | H | Cl | O | C=O | NCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5127 | CH ₂ | H | Cl | O | C=O | NCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 5128 | CH ₂ | H | Cl | O | C=O | NCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 5129 | CH ₂ | H | Cl | O | C=O | NCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 5130 | CH ₂ | H | Cl | O | C=O | NCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 5131 | CH ₂ | H | Cl | O | CCH ₃ | N | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5132 | CH ₂ | H | Cl | O | CCH ₃ | N | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5133 | CH ₂ | H | Cl | O | CCH ₃ | N | CH ₃ | c-C ₃ H ₅ | - |
| 5134 | CH ₂ | H | Cl | O | CCH ₃ | N | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5135 | CH ₂ | H | Cl | O | CCH ₃ | N | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5136 | CH ₂ | H | Cl | O | CCH ₃ | N | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5137 | CH ₂ | H | Cl | O | CCH ₃ | N | C ₂ H ₅ | C ₃ H ₇ | - |
| 5138 | CH ₂ | H | Cl | O | CCH ₃ | N | C ₂ H ₅ | C ₄ H ₉ | - |
| 5139 | CH ₂ | H | Cl | O | CCH ₃ | N | C ₃ H ₇ | C ₃ H ₇ | - |
| 5140 | CH ₂ | H | Cl | O | CCH ₃ | N | CH ₃ | C ₃ H ₇ | - |
| 5141 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5142 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5143 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | CH ₃ | c-C ₃ H ₅ | - |
| 5144 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5145 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5146 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5147 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | C ₂ H ₅ | C ₃ H ₇ | - |
| 5148 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | C ₂ H ₅ | C ₄ H ₉ | - |
| 5149 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | C ₃ H ₇ | C ₃ H ₇ | - |
| 5150 | CH ₂ | H | Cl | O | C=O | NC ₂ H ₅ | CH ₃ | C ₃ H ₇ | - |
| 5151 | CH ₂ | H | Cl | O | C=O | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5152 | CH ₂ | H | Cl | O | C=O | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5153 | CH ₂ | H | Cl | O | C=O | O | CH ₃ | c-C ₃ H ₅ | - |
| 5154 | CH ₂ | H | Cl | O | C=O | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5155 | CH ₂ | H | Cl | O | C=O | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5156 | CH ₂ | H | Cl | O | C=O | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5157 | CH ₂ | H | Cl | O | C=O | O | C ₂ H ₅ | C ₃ H ₇ | - |

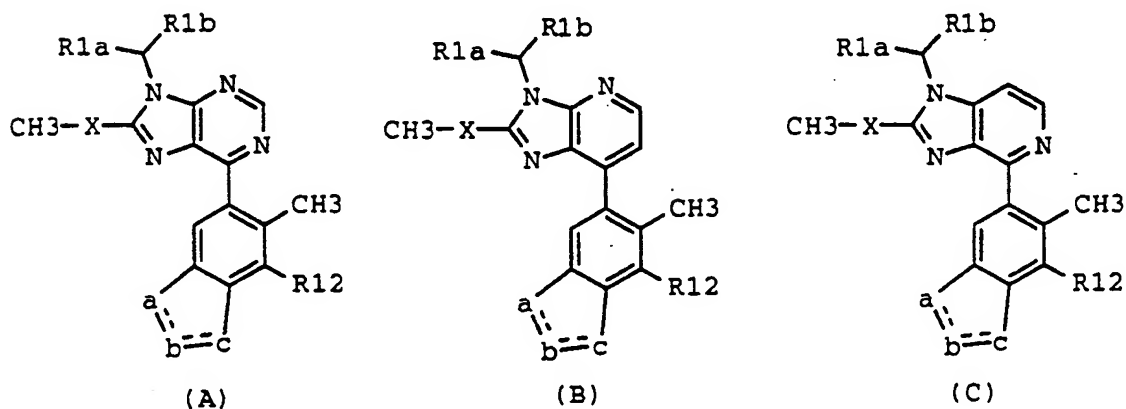
| | | | | | | | | | |
|------|-----------------|---|-----------------|---|---------------------------------|------------------|---------------------------------|---|---|
| 5158 | CH ₂ | H | Cl | O | C=O | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5159 | CH ₂ | H | Cl | O | C=O | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5160 | CH ₂ | H | Cl | O | C=O | O | CH ₃ | C ₃ H ₇ | - |
| 5161 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5162 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5163 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | CH ₃ | c-C ₃ H ₅ | - |
| 5164 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5165 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5166 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5167 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5168 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5169 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5170 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5171 | CH ₂ | H | CH ₃ | O | C=O | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5172 | CH ₂ | H | CH ₃ | O | C=O | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5173 | CH ₂ | H | CH ₃ | O | C=O | O | CH ₃ | c-C ₃ H ₅ | - |
| 5174 | CH ₂ | H | CH ₃ | O | C=O | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5175 | CH ₂ | H | CH ₃ | O | C=O | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5176 | CH ₂ | H | CH ₃ | O | C=O | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5177 | CH ₂ | H | CH ₃ | O | C=O | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5178 | CH ₂ | H | CH ₃ | O | C=O | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5179 | CH ₂ | H | CH ₃ | O | C=O | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5180 | CH ₂ | H | CH ₃ | O | C=O | O | CH ₃ | C ₃ H ₇ | - |
| 5181 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5182 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5183 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | CH ₃ | c-C ₃ H ₅ | - |
| 5184 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5185 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5186 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5187 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5188 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5189 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5190 | CH ₂ | H | CH ₃ | O | CH ₂ CH ₂ | O | CH ₃ | C ₃ H ₇ | - |
| 5191 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5192 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5193 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 5194 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5195 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |

| | | | | | | | | | |
|------|-----------------|---|-----------------|-----------------|---------------------------------|------------------|---------------------------------|---|---------|
| 5196 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5197 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 5198 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 5199 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 5200 | CH ₂ | H | Cl | O | CH ₂ CH ₂ | NCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 5201 | CH ₂ | H | CH ₃ | CH | CH | O | c-C ₃ H ₅ | c-C ₃ H ₅ | 139-141 |
| 5202 | CH ₂ | H | CH ₃ | CH | CH | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5203 | CH ₂ | H | CH ₃ | CH | CH | O | CH ₃ | c-C ₃ H ₅ | - |
| 5204 | CH ₂ | H | CH ₃ | CH | CH | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5205 | CH ₂ | H | CH ₃ | CH | CH | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5206 | CH ₂ | H | CH ₃ | CH | CH | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5207 | CH ₂ | H | CH ₃ | CH | CH | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5208 | CH ₂ | H | CH ₃ | CH | CH | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5209 | CH ₂ | H | CH ₃ | CH | CH | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5210 | CH ₂ | H | CH ₃ | CH | CH | O | CH ₃ | C ₃ H ₇ | - |
| 5211 | CH ₂ | H | Cl | CH | CH | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5212 | CH ₂ | H | Cl | CH | CH | O | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5213 | CH ₂ | H | Cl | CH | CH | O | CH ₃ | c-C ₃ H ₅ | - |
| 5214 | CH ₂ | H | Cl | CH | CH | O | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5215 | CH ₂ | H | Cl | CH | CH | O | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5216 | CH ₂ | H | Cl | CH | CH | O | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5217 | CH ₂ | H | Cl | CH | CH | O | C ₂ H ₅ | C ₃ H ₇ | - |
| 5218 | CH ₂ | H | Cl | CH | CH | O | C ₂ H ₅ | C ₄ H ₉ | - |
| 5219 | CH ₂ | H | Cl | CH | CH | O | C ₃ H ₇ | C ₃ H ₇ | - |
| 5220 | CH ₂ | H | Cl | CH | CH | O | CH ₃ | C ₃ H ₇ | - |
| 5221 | CH ₂ | H | CH ₃ | CH | CHCH | CH | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5222 | CH ₂ | H | CH ₃ | CH | CHCH | CH | H | 4-(CH ₃ O)-C ₆ H ₄ | - |
| 5223 | CH ₂ | H | CH ₃ | CH | CHCH | CH | CH ₃ | c-C ₃ H ₅ | - |
| 5224 | CH ₂ | H | CH ₃ | CH | CHCH | CH | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 5225 | CH ₂ | H | CH ₃ | CH | CHCH | CH | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 5226 | CH ₂ | H | CH ₃ | CH | CHCH | CH | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 5227 | CH ₂ | H | CH ₃ | CH | CHCH | CH | C ₂ H ₅ | C ₃ H ₇ | - |
| 5228 | CH ₂ | H | CH ₃ | CH | CHCH | CH | C ₂ H ₅ | C ₄ H ₉ | - |
| 5229 | CH ₂ | H | CH ₃ | CH | CHCH | CH | C ₃ H ₇ | C ₃ H ₇ | - |
| 5230 | CH ₂ | H | CH ₃ | CH | CHCH | CH | CH ₃ | C ₃ H ₇ | - |
| 5231 | CH ₂ | H | CH ₃ | CH | CBr | O | c-C ₃ H ₅ | c-C ₃ H ₅ | 177-178 |
| 5232 | CH ₂ | H | CH ₃ | CH ₂ | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | 179-180 |
| 5233 | CH ₂ | H | CH ₃ | CH | CCH ₃ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |

| | | | | | | | | | |
|------|-----------------|---|-----------------|-----------------|--------------------|---|---------------------------------|---------------------------------|---|
| 5234 | CH ₂ | H | CH ₃ | CH ₂ | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5235 | CH ₂ | H | CH ₃ | CH | CSCCH ₃ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5236 | CH ₂ | H | CH ₃ | CH ₂ | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |

5

TABLE 5A



10

| Ex. No. | X | R ¹² | a | b | c | R ^{1a} | R ^{1b} | m.p., °C |
|---------|-----------------|------------------|-----------------|-----------------|---|---------------------------------|---------------------------------|----------|
| 5232 | CH ₂ | Br | CH ₂ | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | 179-180 |
| 5234 | CH ₂ | CN | CH ₂ | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 5236 | CH ₂ | SCH ₃ | CH ₂ | CH ₂ | O | c-C ₃ H ₅ | c-C ₃ H ₅ | - |

15

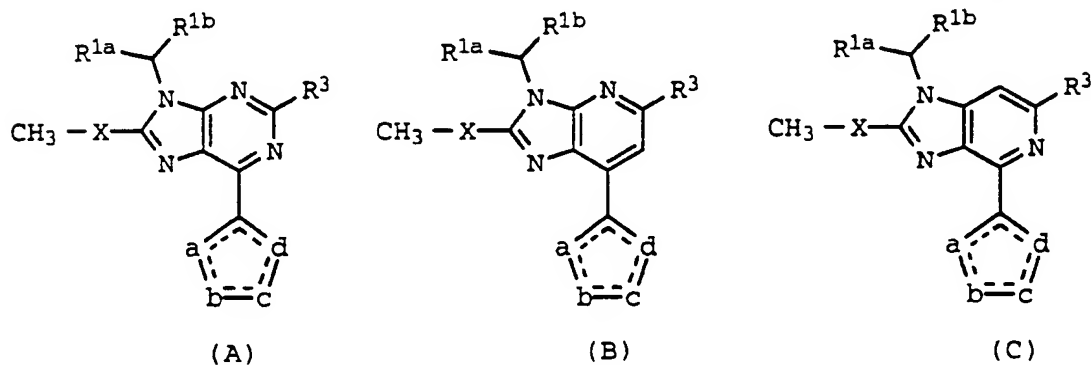
The methods used in the preparation of the compounds of Table 1 may be used for the compounds of Structure A of Table 6. For example, replacing variously-substituted pentaatomic heteroaryl boronic acids for benzenboronic acids in the palladium-catalyzed aryl cross-coupling method (see Examples 35 or 831) will afford the desired 6-heteroarylpyrine compounds.

20

The methods of Schemes 13 and 14 may be used to prepare many of the examples of Structure B and Structure C contained in Table 6, with minor procedural modifications where necessary and use of reagents of the appropriate structure.

TABLE 6

10



| Ex. No. | X | R ³ | a | b | c | d | R ^{1a} | R ^{1b} | m.p. °C * |
|---------|-----------------|----------------|------------------|---|---|------------------|---------------------------------|---|--------------|
| 6001 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | oil |
| 6002 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6003 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6004 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6005 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6006 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6007 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6008 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6009 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6010 | CH ₂ | H | CCH ₃ | N | O | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6011 | O | H | CCH ₃ | N | O | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6012 | O | H | CCH ₃ | N | O | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6013 | O | H | CCH ₃ | N | O | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |

| | | | | | | | | | |
|------|-----------------|-----------------|------------------|---|------------------|------------------|---------------------------------|---|---|
| 6014 | O | H | CCH ₃ | N | O | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6015 | O | H | CCH ₃ | N | O | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6016 | O | H | CCH ₃ | N | O | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6017 | O | H | CCH ₃ | N | O | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6018 | O | H | CCH ₃ | N | O | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6019 | O | H | CCH ₃ | N | O | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6020 | O | H | CCH ₃ | N | O | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6021 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6022 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6023 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6024 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6025 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6026 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6027 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6028 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6029 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6030 | CH ₂ | CH ₃ | CCH ₃ | N | O | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6031 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6032 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6033 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6034 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6035 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6036 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6037 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6038 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6039 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6040 | CH ₂ | H | CCH ₃ | N | NCH ₃ | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6041 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6042 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6043 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6044 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6045 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6046 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6047 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6048 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6049 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6050 | O | H | CCH ₃ | N | NCH ₃ | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6051 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |

| | | | | | | | | | |
|------|-----------------|-----------------|------------------|---|--------------------------------|------------------|---------------------------------|---|---|
| 6052 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6053 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6054 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6055 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6056 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6057 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6058 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6059 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6060 | CH ₂ | CH ₃ | CCH ₃ | N | NCH ₃ | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6061 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6062 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6063 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6064 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6065 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6066 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6067 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6068 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6069 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6070 | CH ₂ | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6071 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6072 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6073 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6074 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6075 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6076 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6077 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6078 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6079 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6080 | O | H | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6081 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6082 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6083 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6084 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6085 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6086 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6087 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6088 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6089 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |

| | | | | | | | | | |
|------|-----------------|-----------------|------------------|---|--------------------------------|------------------|---------------------------------|---|---|
| 6090 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₂ H ₅ | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6091 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6092 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6093 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6094 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6095 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6096 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6097 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6098 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6099 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6100 | CH ₂ | H | CCH ₃ | N | CCH ₃ | NCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6101 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6102 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6103 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6104 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6105 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6106 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6107 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6108 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6109 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6110 | CH ₂ | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6111 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6112 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6113 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6114 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6115 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6116 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6117 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |
| 6118 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6119 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6120 | O | H | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |
| 6121 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | c-C ₃ H ₅ | c-C ₃ H ₅ | - |
| 6122 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | CH ₃ | c-C ₃ H ₅ | - |
| 6123 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₂ H ₅ | c-C ₃ H ₅ | - |
| 6124 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₃ H ₇ | c-C ₃ H ₅ | - |
| 6125 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₄ H ₉ | c-C ₃ H ₅ | - |
| 6126 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | CH ₃ | C ₃ H ₇ | - |
| 6127 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₂ H ₅ | C ₃ H ₇ | - |

| | | | | | | | | | |
|------|-----------------|-----------------|------------------|---|--------------------------------|------------------|-------------------------------|---|---|
| 6128 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₃ H ₇ | C ₃ H ₇ | - |
| 6129 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | C ₂ H ₅ | C ₄ H ₉ | - |
| 6130 | CH ₂ | CH ₃ | CCH ₃ | N | NC ₆ H ₅ | CCH ₃ | H | 4-CH ₃ O-C ₆ H ₄ | - |

Key:

a) Where the compound is indicated as an "oil", spectral data is provided as follows:

5 Example 6001 spectral data: MS (NH₃-CI): m/e 338 (M+H⁺, 100%).

10 The methods used in the preparation of the compounds of Table 1 may be used for preparation of many of the compounds of Structure A of Table 7. The preparation of those compounds derived from cycloaddition of compounds with alkynyl-bearing R¹ groups is illustrated by the following examples.

15 The methods of Schemes 13 and 14 may be used to prepare many of the examples of Structure B and Structure C contained in Table 7, with minor procedural modifications where necessary and use of reagents of the appropriate structure.

20

Example 7409

Preparation of 9-[1-cyclopropyl-1-(3-methyl-isoxazol-5-yl)methyl]-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine

25 To a stirring solution of the compound of Example 7241 (90 mg, 0.24 mmol; prepared in a manner similar to that of Example 2 using 6-(2,4-dichlorophenyl)-8-ethyl-9H-purine and 3-cyclopropyl-1-propyn-3-ol) in methylene chloride (2 mL) were added chloroacetaldoxime (25 mg, 0.27 mmol) and triethylamine (0.038 mL, 0.27 mmol). (The chloroacetaldoxime used was
30 previously prepared by reacting equimolar amounts of acetaldoxime and N-chlorosuccinimide in DMF, then extracting the product into diethyl ether and washing with water.) The cycloaddition reaction was monitored by TLC and additional amounts of chloroacetaldoxime and triethylamine were added

until all the starting material was consumed. The reaction mixture was purified by adding directly to a column packed with silica gel and eluting using a gradient of 100% hexane to 25% ethyl acetate in hexane. 72 mg of a white foam was
5 collected. MS (NH₃-CI) 428 (M+H⁺). HRMS: m/e = 428.1037 (M+H⁺, C₂₁H₂₀Cl₂N₅O). Purity by reverse phase HPLC >97%.

Examples 7396 and 7398

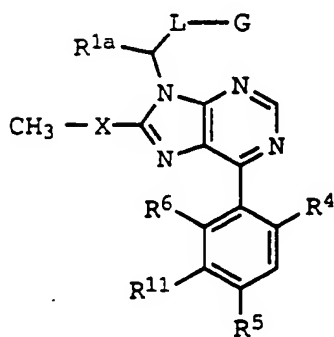
Preparation of 6-(2,4-dichlorophenyl)-9-[1-(3-ethoxycarbonyl- 10 isoxazol-5-yl)butyl]-8-ethyl-9H-purine and 9-[1-(4-cyano-3-ethoxycarbonyl-isoxazol-5-yl)butyl]-6-(2,4-dichlorophenyl)-8-ethyl-9H-purine

A solution of the compound of Example 7259 (120 mg, 0.321 mmol; prepared prepared in a manner similar to that of Example
15 2 using 6-(2,4-dichlorophenyl)-8-ethyl-9H-purine and 1-hexyn-3-ol), ethyl chlorooximidoacetate (146 mg, 0.963 mmol) and diisopropylethylamine (170 µL, 0.976 mmol) in toluene (2 mL) was heated to reflux for 20 hours, then cooled and diluted with 20 mL ethyl acetate. This was washed with water (2 x 20
20 mL) and satd. aq. brine (20 mL), and the aqueous phases were back-extracted in sequence with ethyl acetate (20 mL). The organic extracts were combined, dried over anhydrous sodium sulfate, filtered and evaporated. The residual material was separated by column chromatography (silica gel, 1:4 ethyl
25 acetate-hexane) to afford, in order, unreacted starting material (about 50 mg), then the compound of Example 7396 (58.7 mg, 0.120 mmol, 37%), and finally the compound of Example 7398 (23.8 mg, 0.046 mmol, 14%), the latter two compounds being amorphous solids. Example 7396 spectral data:
30 TLC R_f 0.27 (20:80 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.96 (1H, s), 7.67 (1H, d, J = 8.1 Hz), 7.58 (1H, d, J = 1.8 Hz), 7.41 (1H, dd, J = 8.1, 1.8 Hz), 6.86 (1H, s), 5.83 (1H, dd, J = 9.9, 6.2 Hz), 4.43 (2H, q, J = 7.3 Hz), 2.98 (2H, q, J = 7.7 Hz), 2.91-2.78 (1H, m), 2.63-2.49 (1H, m),
35 1.42 (3H, t, J = 7.7 Hz), 1.40 (3H, t, J = 7.3 Hz), 1.39-1.19 (2H, m), 1.00 (3H, t, J = 7.3 Hz). MS (NH₃-CI): m/e calc'd for C₂₃H₂₄Cl₂N₅O₃: 488.1256, found 488.1252; 493 (3), 492 (13), 491

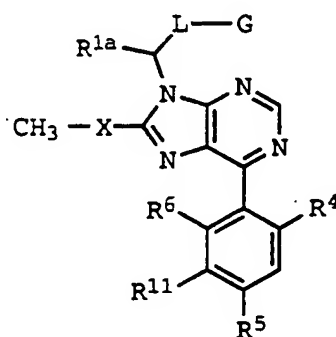
(18), 490 (68), 489 (28), 488 (100). Example 7398 spectral data: TLC R_f 0.11 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.99 (1H, s), 7.72 (1H, d, $J = 8.1$ Hz), 7.59 (1H, d, $J = 1.8$ Hz), 7.42 (1H, dd, $J = 8.1, 1.8$ Hz), 5.40 (1H, dd, $J = 10.4, 5.0$ Hz), 4.42 (2H, q, $J = 7.4$ Hz), 3.00-2.90 (2H, m), 2.66-2.52 (1H, m), 2.51-2.38 (1H, m), 1.46 (3H, t, $J = 7.4$ Hz), 1.41 (3H, t, $J = 7.3$ Hz), 1.40-1.10 (2H, m), 0.98 (3H, t, $J = 7.2$ Hz). MS (NH_3 -CI): m/e calc'd for $\text{C}_{24}\text{H}_{25}\text{Cl}_2\text{N}_6\text{O}_4$: 531.1315, found 531.1315; 531 (100).

10

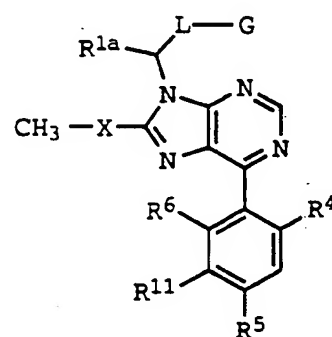
TABLE 7



(A)



(B)



(C)

15

| Ex. No. | X | R ⁴ | R ⁵ | R ¹¹ | R ⁶ | R ^{1a} | L | G ^a | m.p., °C ^b |
|---------|-----------------|-----------------|-----------------|-----------------|-----------------|---|------|----------------|--------------------------|
| 7001 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | bond | G1 | - |
| 7002 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | bond | G1 | - |
| 7003 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | bond | G1 | - |
| 7004 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | <i>c</i> -C ₃ H ₅ | bond | G1 | - |
| 7005 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | bond | G2 | - |
| 7006 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | bond | G2 | - |
| 7007 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | bond | G2 | - |
| 7008 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | <i>c</i> -C ₃ H ₅ | bond | G2 | - |
| 7009 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | bond | G3 | - |
| 7010 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | bond | G3 | - |
| 7011 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | bond | G3 | - |

| | | | | | | | | | |
|------|-----------------|-----------------|-----------------|---|-----------------|---------------------------------|-----------------|----|---|
| 7012 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | bond | G3 | - |
| 7013 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | CH ₂ | G4 | - |
| 7014 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ | G4 | - |
| 7015 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | CH ₂ | G4 | - |
| 7016 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | CH ₂ | G4 | - |
| 7017 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | CH ₂ | G5 | - |
| 7018 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ | G5 | - |
| 7019 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | CH ₂ | G5 | - |
| 7020 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | CH ₂ | G5 | - |
| 7021 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | bond | G6 | - |
| 7022 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | bond | G6 | - |
| 7023 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | bond | G6 | - |
| 7024 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | c-C ₃ H ₅ | bond | G6 | - |
| 7025 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | CH ₂ =CH | bond | G7 | - |
| 7026 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | CH ₃ | bond | G8 | - |
| 7027 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ | G1 | - |
| 7028 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | CH ₂ | G1 | - |
| 7029 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ | G2 | - |
| 7030 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₃ H ₇ | CH ₂ | G2 | - |
| 7031 | CH ₂ | Cl | Cl | H | H | CH ₃ | bond | G1 | - |
| 7032 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | bond | G1 | - |
| 7033 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | bond | G1 | - |
| 7034 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G1 | - |
| 7035 | CH ₂ | Cl | Cl | H | H | CH ₃ | bond | G2 | - |
| 7036 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | bond | G2 | - |
| 7037 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | bond | G2 | - |
| 7038 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G2 | - |
| 7039 | CH ₂ | Cl | Cl | H | H | CH ₃ | bond | G3 | - |
| 7040 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | bond | G3 | - |
| 7041 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | bond | G3 | - |
| 7042 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G3 | - |
| 7043 | CH ₂ | Cl | Cl | H | H | CH ₃ | CH ₂ | G4 | - |
| 7044 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7045 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | CH ₂ | G4 | - |
| 7046 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | CH ₂ | G4 | - |
| 7047 | CH ₂ | Cl | Cl | H | H | CH ₃ | CH ₂ | G5 | - |
| 7048 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ | G5 | - |
| 7049 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | CH ₂ | G5 | - |

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|------|-----------------|-----------------|------------------|---|---|---------------------------------|-----------------|----|-----|
| 7050 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | CH ₂ | G5 | - |
| 7051 | CH ₂ | Cl | Cl | H | H | CH ₃ | bond | G6 | - |
| 7052 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | bond | G6 | - |
| 7053 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | bond | G6 | - |
| 7054 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G6 | - |
| 7055 | CH ₂ | Cl | Cl | H | H | CH ₂ =CH | bond | G7 | - |
| 7056 | CH ₂ | Cl | Cl | H | H | CH ₃ | bond | G8 | - |
| 7057 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ | G1 | - |
| 7058 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7059 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | CH ₂ | G2 | - |
| 7060 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | CH ₂ | G2 | - |
| 7061 | CH ₂ | CH ₃ | OCH ₃ | H | H | CH ₃ | bond | G1 | - |
| 7062 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | bond | G1 | - |
| 7063 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | bond | G1 | - |
| 7064 | CH ₂ | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G1 | - |
| 7065 | CH ₂ | CH ₃ | OCH ₃ | H | H | CH ₃ | bond | G2 | - |
| 7066 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | bond | G2 | - |
| 7067 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | bond | G2 | - |
| 7068 | CH ₂ | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G2 | - |
| 7069 | CH ₂ | CH ₃ | OCH ₃ | H | H | CH ₃ | bond | G3 | - |
| 7070 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | bond | G3 | - |
| 7071 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | bond | G3 | - |
| 7072 | CH ₂ | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G3 | - |
| 7073 | CH ₂ | CH ₃ | OCH ₃ | H | H | CH ₃ | CH ₂ | G4 | - |
| 7074 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7075 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | CH ₂ | G4 | - |
| 7076 | CH ₂ | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | CH ₂ | G4 | - |
| 7077 | CH ₂ | CH ₃ | OCH ₃ | H | H | CH ₃ | CH ₂ | G5 | - |
| 7078 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ | G5 | - |
| 7079 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | CH ₂ | G5 | - |
| 7080 | CH ₂ | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | CH ₂ | G5 | - |
| 7081 | CH ₂ | CH ₃ | OCH ₃ | H | H | CH ₃ | bond | G6 | - |
| 7082 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | bond | G6 | - |
| 7083 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | bond | G6 | - |
| 7084 | CH ₂ | CH ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G6 | - |
| 7085 | CH ₂ | CH ₃ | OCH ₃ | H | H | CH ₂ =CH | bond | G7 | - |
| 7086 | CH ₂ | CH ₃ | OCH ₃ | H | H | CH ₃ | bond | G8 | oil |
| 7087 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ | G1 | - |

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|------|-----------------|-----------------|------------------|---|---|---------------------------------|-----------------|----|-----|
| 7088 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7089 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ | G2 | - |
| 7090 | CH ₂ | CH ₃ | OCH ₃ | H | H | C ₃ H ₇ | CH ₂ | G2 | - |
| 7091 | CH ₂ | Cl | OCH ₃ | H | H | CH ₃ | bond | G1 | - |
| 7092 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | bond | G1 | - |
| 7093 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | bond | G1 | - |
| 7094 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G1 | - |
| 7095 | CH ₂ | Cl | OCH ₃ | H | H | CH ₃ | bond | G2 | - |
| 7096 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | bond | G2 | - |
| 7097 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | bond | G2 | - |
| 7098 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G2 | - |
| 7099 | CH ₂ | Cl | OCH ₃ | H | H | CH ₃ | bond | G3 | - |
| 7100 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | bond | G3 | - |
| 7101 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | bond | G3 | - |
| 7102 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G3 | - |
| 7103 | CH ₂ | Cl | OCH ₃ | H | H | CH ₃ | CH ₂ | G4 | - |
| 7104 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7105 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | CH ₂ | G4 | - |
| 7106 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | CH ₂ | G4 | - |
| 7107 | CH ₂ | Cl | OCH ₃ | H | H | CH ₃ | CH ₂ | G5 | - |
| 7108 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ | G5 | - |
| 7109 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | CH ₂ | G5 | - |
| 7110 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | CH ₂ | G5 | - |
| 7111 | CH ₂ | Cl | OCH ₃ | H | H | CH ₃ | bond | G6 | - |
| 7112 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | bond | G6 | - |
| 7113 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | bond | G6 | - |
| 7114 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G6 | - |
| 7115 | CH ₂ | Cl | OCH ₃ | H | H | CH ₂ =CH | bond | G7 | - |
| 7116 | CH ₂ | Cl | OCH ₃ | H | H | CH ₃ | bond | G8 | oil |
| 7117 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ | G1 | - |
| 7118 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7119 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | CH ₂ | G2 | - |
| 7120 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | CH ₂ | G2 | - |
| 7121 | CH ₂ | Cl | CF ₃ | H | H | CH ₃ | bond | G1 | - |
| 7122 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G1 | - |
| 7123 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G1 | - |
| 7124 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G1 | - |
| 7125 | CH ₂ | Cl | CF ₃ | H | H | CH ₃ | bond | G2 | - |

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|------|-----------------|-----------------|-----------------|---|---|---------------------------------|-----------------|----|-----|
| 7126 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G2 | - |
| 7127 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G2 | - |
| 7128 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G2 | - |
| 7129 | CH ₂ | Cl | CF ₃ | H | H | CH ₃ | bond | G3 | - |
| 7130 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G3 | - |
| 7131 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G3 | - |
| 7132 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G3 | - |
| 7133 | CH ₂ | Cl | CF ₃ | H | H | CH ₃ | CH ₂ | G4 | - |
| 7134 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7135 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | CH ₂ | G4 | - |
| 7136 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | CH ₂ | G4 | - |
| 7137 | CH ₂ | Cl | CF ₃ | H | H | CH ₃ | CH ₂ | G5 | - |
| 7138 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ | G5 | - |
| 7139 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | CH ₂ | G5 | - |
| 7140 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | CH ₂ | G5 | - |
| 7141 | CH ₂ | Cl | CF ₃ | H | H | CH ₃ | bond | G6 | - |
| 7142 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G6 | - |
| 7143 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G6 | - |
| 7144 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G6 | - |
| 7145 | CH ₂ | Cl | CF ₃ | H | H | CH ₂ =CH | bond | G7 | - |
| 7146 | CH ₂ | Cl | CF ₃ | H | H | CH ₃ | bond | G8 | oil |
| 7147 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ | G1 | - |
| 7148 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7149 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ | G2 | - |
| 7150 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | CH ₂ | G2 | - |
| 7151 | CH ₂ | CF ₃ | Cl | H | H | CH ₃ | bond | G1 | - |
| 7152 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | bond | G1 | - |
| 7153 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | bond | G1 | - |
| 7154 | CH ₂ | CF ₃ | Cl | H | H | c-C ₃ H ₅ | bond | G1 | - |
| 7155 | CH ₂ | CF ₃ | Cl | H | H | CH ₃ | bond | G2 | - |
| 7156 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | bond | G2 | - |
| 7157 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | bond | G2 | - |
| 7158 | CH ₂ | CF ₃ | Cl | H | H | c-C ₃ H ₅ | bond | G2 | - |
| 7159 | CH ₂ | CF ₃ | Cl | H | H | CH ₃ | bond | G3 | - |
| 7160 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | bond | G3 | - |
| 7161 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | bond | G3 | - |
| 7162 | CH ₂ | CF ₃ | Cl | H | H | c-C ₃ H ₅ | bond | G3 | - |
| 7163 | CH ₂ | CF ₃ | Cl | H | H | CH ₃ | CH ₂ | G4 | - |

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|------|-----------------|-----------------|------------------|-----------------|---|---------------------------------|-----------------|----|---|
| 7164 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7165 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | CH ₂ | G4 | - |
| 7166 | CH ₂ | CF ₃ | Cl | H | H | c-C ₃ H ₅ | CH ₂ | G4 | - |
| 7167 | CH ₂ | CF ₃ | Cl | H | H | CH ₃ | CH ₂ | G5 | - |
| 7168 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | CH ₂ | G5 | - |
| 7169 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | CH ₂ | G5 | - |
| 7170 | CH ₂ | CF ₃ | Cl | H | H | c-C ₃ H ₅ | CH ₂ | G5 | - |
| 7171 | CH ₂ | CF ₃ | Cl | H | H | CH ₃ | bond | G6 | - |
| 7172 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | bond | G6 | - |
| 7173 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | bond | G6 | - |
| 7174 | CH ₂ | CF ₃ | Cl | H | H | c-C ₃ H ₅ | bond | G6 | - |
| 7175 | CH ₂ | CF ₃ | Cl | H | H | CH ₂ =CH | bond | G7 | - |
| 7176 | CH ₂ | CF ₃ | Cl | H | H | CH ₃ | bond | G8 | - |
| 7177 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | CH ₂ | G1 | - |
| 7178 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7179 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | CH ₂ | G2 | - |
| 7180 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | CH ₂ | G2 | - |
| 7181 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | bond | G1 | - |
| 7182 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | bond | G1 | - |
| 7183 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | bond | G1 | - |
| 7184 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₃ H ₅ | bond | G1 | - |
| 7185 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | bond | G2 | - |
| 7186 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | bond | G2 | - |
| 7187 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | bond | G2 | - |
| 7188 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₃ H ₅ | bond | G2 | - |
| 7189 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | bond | G3 | - |
| 7190 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | bond | G3 | - |
| 7191 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | bond | G3 | - |
| 7192 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₃ H ₅ | bond | G3 | - |
| 7193 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | CH ₂ | G4 | - |
| 7194 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7195 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | CH ₂ | G4 | - |
| 7196 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₃ H ₅ | CH ₂ | G4 | - |
| 7197 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | CH ₂ | G5 | - |
| 7198 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | CH ₂ | G5 | - |
| 7199 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | CH ₂ | G5 | - |
| 7200 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₃ H ₅ | CH ₂ | G5 | - |
| 7201 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | bond | G6 | - |

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|------|-----------------|-----------------|------------------|-----------------|-----------------|---------------------------------|-------------------|----|-----|
| 7202 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | bond | G6 | - |
| 7203 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | bond | G6 | - |
| 7204 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | c-C ₃ H ₅ | bond | G6 | - |
| 7205 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₂ =CH | bond | G7 | - |
| 7206 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | bond | G8 | - |
| 7207 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | CH ₂ | G1 | - |
| 7208 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7209 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₂ H ₅ | CH ₂ | G2 | - |
| 7210 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | CH ₂ | G2 | - |
| 7211 | O | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ | G1 | - |
| 7212 | O | Cl | CF ₃ | H | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7213 | O | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G2 | - |
| 7214 | O | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G2 | - |
| 7215 | O | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7216 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ | G1 | - |
| 7217 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7218 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G2 | - |
| 7219 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G2 | - |
| 7220 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7221 | O | CF ₃ | Cl | H | H | C ₂ H ₅ | CH ₂ | G1 | - |
| 7222 | O | CF ₃ | Cl | H | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7223 | O | CF ₃ | Cl | H | H | C ₂ H ₅ | bond | G2 | - |
| 7224 | O | CF ₃ | Cl | H | H | C ₃ H ₇ | bond | G2 | - |
| 7225 | O | CF ₃ | Cl | H | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7226 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | CH ₂ | G1 | - |
| 7227 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | CH ₂ | G1 | - |
| 7228 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | bond | G2 | - |
| 7229 | CH ₂ | CF ₃ | Cl | H | H | C ₃ H ₇ | bond | G2 | - |
| 7230 | CH ₂ | CF ₃ | Cl | H | H | C ₂ H ₅ | CH ₂ | G4 | - |
| 7231 | CH ₂ | CH ₃ | CH ₃ | H | CH ₃ | C ₂ H ₅ | CH ₂ O | G3 | oil |
| 7232 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G9 | - |
| 7233 | O | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G9 | - |
| 7234 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G9 | oil |
| 7235 | O | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G9 | - |
| 7236 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G9 | - |
| 7237 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₃ H ₅ | bond | G9 | - |
| 7238 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₃ H ₅ | bond | G9 | - |
| 7239 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₃ H ₅ | bond | G9 | - |

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|------|-----------------|-----------------|------------------|----|-----------------|---------------------------------|-----------------|-----|-------|
| 7240 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G9 | - |
| 7241 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G10 | oil |
| 7242 | O | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G10 | - |
| 7243 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G10 | oil |
| 7244 | O | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G10 | - |
| 7245 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G10 | - |
| 7246 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₃ H ₅ | bond | G10 | - |
| 7247 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₃ H ₅ | bond | G10 | - |
| 7248 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₃ H ₅ | bond | G10 | - |
| 7249 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G10 | oil |
| 7250 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | bond | G10 | oil |
| 7251 | O | Cl | Cl | H | H | C ₂ H ₅ | bond | G10 | - |
| 7252 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G10 | 98-99 |
| 7253 | O | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G10 | - |
| 7254 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | bond | G10 | - |
| 7255 | CH ₂ | Cl | OCF ₃ | H | H | C ₂ H ₅ | bond | G10 | - |
| 7256 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | bond | G10 | - |
| 7257 | CH ₂ | Cl | Cl | H | CH ₃ | C ₂ H ₅ | bond | G10 | - |
| 7258 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₂ H ₅ | bond | G10 | - |
| 7259 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | bond | G10 | oil |
| 7260 | O | Cl | Cl | H | H | C ₃ H ₇ | bond | G10 | - |
| 7261 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G10 | oil |
| 7262 | O | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G10 | - |
| 7263 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | bond | G10 | - |
| 7264 | CH ₂ | Cl | OCF ₃ | H | H | C ₃ H ₇ | bond | G10 | - |
| 7265 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₃ H ₇ | bond | G10 | - |
| 7266 | CH ₂ | Cl | Cl | H | CH ₃ | C ₃ H ₇ | bond | G10 | oil |
| 7267 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₃ H ₇ | bond | G10 | - |
| 7268 | CH ₂ | Cl | Cl | H | H | C ₅ H ₁₁ | bond | G10 | oil |
| 7269 | O | Cl | Cl | H | H | C ₅ H ₁₁ | bond | G10 | - |
| 7270 | CH ₂ | Cl | CF ₃ | H | H | C ₅ H ₁₁ | bond | G10 | oil |
| 7271 | O | Cl | CF ₃ | H | H | C ₅ H ₁₁ | bond | G10 | - |
| 7272 | CH ₂ | Cl | OCH ₃ | H | H | C ₅ H ₁₁ | bond | G10 | - |
| 7273 | CH ₂ | Cl | OCF ₃ | H | H | C ₅ H ₁₁ | bond | G10 | - |
| 7274 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₅ H ₁₁ | bond | G10 | - |
| 7275 | CH ₂ | Cl | Cl | H | CH ₃ | C ₅ H ₁₁ | bond | G10 | - |
| 7276 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₅ H ₁₁ | bond | G10 | - |
| 7277 | CH ₂ | Cl | Cl | H | H | CH ₃ | CH ₂ | G10 | - |

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|------|-----------------|-----------------|------------------|----|-----------------|---------------------------------|-----------------|-----|---------|
| 7278 | O | Cl | Cl | H | H | CH ₃ | CH ₂ | G10 | - |
| 7279 | CH ₂ | Cl | CF ₃ | H | H | CH ₃ | CH ₂ | G10 | oil |
| 7280 | O | Cl | CF ₃ | H | H | CH ₃ | CH ₂ | G10 | - |
| 7281 | CH ₂ | Cl | OCH ₃ | H | H | CH ₃ | CH ₂ | G10 | - |
| 7282 | CH ₂ | Cl | OCF ₃ | H | H | CH ₃ | CH ₂ | G10 | - |
| 7283 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | CH ₃ | CH ₂ | G10 | - |
| 7284 | CH ₂ | Cl | Cl | H | CH ₃ | CH ₃ | CH ₂ | G10 | - |
| 7285 | CH ₂ | CF ₃ | OCH ₃ | H | H | CH ₃ | CH ₂ | G10 | - |
| 7286 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G11 | oil |
| 7287 | O | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G11 | - |
| 7288 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G11 | oil |
| 7289 | O | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G11 | - |
| 7290 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G11 | - |
| 7291 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₃ H ₅ | bond | G11 | - |
| 7292 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₃ H ₅ | bond | G11 | - |
| 7293 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₃ H ₅ | bond | G11 | - |
| 7294 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G11 | - |
| 7295 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | bond | G11 | oil |
| 7296 | O | Cl | Cl | H | H | C ₂ H ₅ | bond | G11 | - |
| 7297 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G11 | oil |
| 7298 | O | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G11 | - |
| 7299 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | bond | G11 | - |
| 7300 | CH ₂ | Cl | OCF ₃ | H | H | C ₂ H ₅ | bond | G11 | - |
| 7301 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | bond | G11 | - |
| 7302 | CH ₂ | Cl | Cl | H | CH ₃ | C ₂ H ₅ | bond | G11 | - |
| 7303 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₂ H ₅ | bond | G11 | - |
| 7304 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | bond | G11 | 88-89 |
| 7305 | O | Cl | Cl | H | H | C ₃ H ₇ | bond | G11 | - |
| 7306 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G11 | oil |
| 7307 | O | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G11 | - |
| 7308 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | bond | G11 | - |
| 7309 | CH ₂ | Cl | OCF ₃ | H | H | C ₃ H ₇ | bond | G11 | - |
| 7310 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₃ H ₇ | bond | G11 | - |
| 7311 | CH ₂ | Cl | Cl | H | CH ₃ | C ₃ H ₇ | bond | G11 | - |
| 7312 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₃ H ₇ | bond | G11 | - |
| 7313 | CH ₂ | Cl | Cl | H | H | C ₆ H ₅ | bond | G11 | 156-157 |
| 7314 | O | Cl | Cl | H | H | C ₆ H ₅ | bond | G11 | - |
| 7315 | CH ₂ | Cl | CF ₃ | H | H | C ₆ H ₅ | bond | G11 | 150-151 |

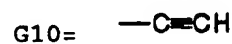
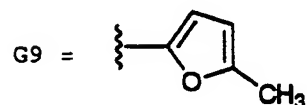
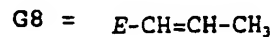
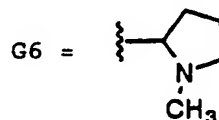
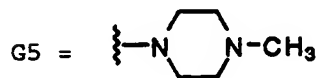
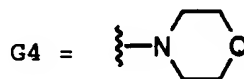
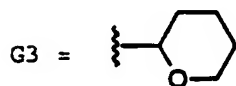
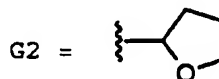
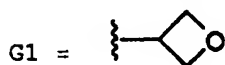
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|------|-----------------|-----------------|------------------|----|-----------------|---------------------------------|------|-----|---------|
| 7316 | O | Cl | CF ₃ | H | H | C ₆ H ₅ | bond | G11 | - |
| 7317 | CH ₂ | Cl | OCH ₃ | H | H | C ₆ H ₅ | bond | G11 | - |
| 7318 | CH ₂ | Cl | OCF ₃ | H | H | C ₆ H ₅ | bond | G11 | - |
| 7319 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₆ H ₅ | bond | G11 | - |
| 7320 | CH ₂ | Cl | Cl | H | CH ₃ | C ₆ H ₅ | bond | G11 | - |
| 7321 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₆ H ₅ | bond | G11 | - |
| 7322 | CH ₂ | Cl | Cl | H | H | C ₂ H ₅ | bond | G12 | - |
| 7323 | O | Cl | Cl | H | H | C ₂ H ₅ | bond | G12 | - |
| 7324 | CH ₂ | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G12 | oil |
| 7325 | O | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G12 | - |
| 7326 | CH ₂ | Cl | OCH ₃ | H | H | C ₂ H ₅ | bond | G12 | - |
| 7327 | CH ₂ | Cl | OCF ₃ | H | H | C ₂ H ₅ | bond | G12 | - |
| 7328 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | bond | G12 | - |
| 7329 | CH ₂ | Cl | Cl | H | CH ₃ | C ₂ H ₅ | bond | G12 | - |
| 7330 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₂ H ₅ | bond | G12 | - |
| 7331 | CH ₂ | Cl | Cl | H | H | C ₃ H ₇ | bond | G12 | - |
| 7332 | O | Cl | Cl | H | H | C ₃ H ₇ | bond | G12 | - |
| 7333 | CH ₂ | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G12 | - |
| 7334 | O | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G12 | - |
| 7335 | CH ₂ | Cl | OCH ₃ | H | H | C ₃ H ₇ | bond | G12 | - |
| 7336 | CH ₂ | Cl | OCF ₃ | H | H | C ₃ H ₇ | bond | G12 | - |
| 7337 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₃ H ₇ | bond | G12 | - |
| 7338 | CH ₂ | Cl | Cl | H | CH ₃ | C ₃ H ₇ | bond | G12 | - |
| 7339 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₃ H ₇ | bond | G12 | - |
| 7340 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G12 | - |
| 7341 | O | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G12 | - |
| 7342 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G12 | 128-130 |
| 7343 | O | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G12 | - |
| 7344 | CH ₂ | Cl | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G12 | - |
| 7345 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₃ H ₅ | bond | G12 | - |
| 7346 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₃ H ₅ | bond | G12 | - |
| 7347 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₃ H ₅ | bond | G12 | - |
| 7348 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G12 | - |
| 7349 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G13 | oil |
| 7350 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G13 | - |
| 7351 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G7 | oil |
| 7352 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G7 | oil |
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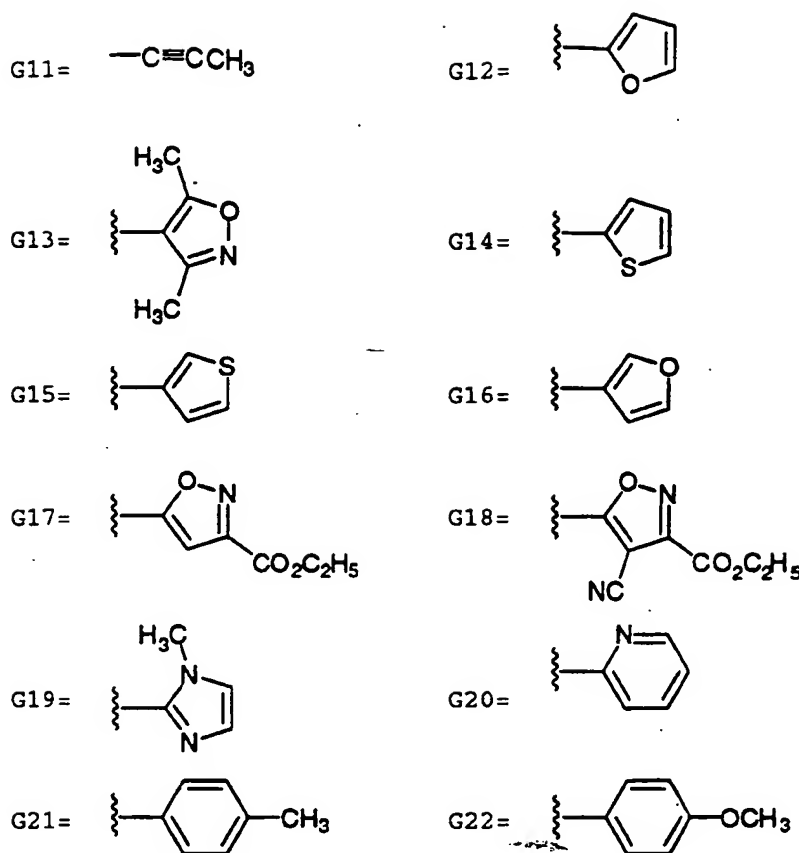
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|------|-----------------|-----------------|------------------|------------------|-----------------|---------------------------------|------|-----|---------|
| 7354 | CH ₂ | Cl | Cl | H | H | CH ₃ | bond | G7 | - |
| 7355 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | CH ₃ | bond | G7 | oil |
| 7356 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₃ H ₇ | bond | G7 | oil |
| 7357 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₃ H ₇ | bond | G7 | oil |
| 7358 | CH ₂ | CH ₃ | OCH ₃ | CH ₃ | H | C ₄ H ₉ | bond | G7 | oil |
| 7359 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₃ H ₅ | bond | G7 | 156-158 |
| 7360 | CH ₂ | CF ₃ | OCH ₃ | H | H | CH ₃ | bond | G8 | oil |
| 7361 | CH ₂ | CH ₃ | OCH ₃ | OCH ₃ | H | C ₂ H ₅ | bond | G10 | oil |
| 7362 | O | Cl | Cl | H | H | CH ₃ | bond | G1 | - |
| 7363 | O | Cl | CF ₃ | H | H | CH ₃ | bond | G1 | - |
| 7364 | CH ₂ | Cl | OCF ₃ | H | H | CH ₃ | bond | G1 | - |
| 7365 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | CH ₃ | bond | G1 | - |
| 7366 | CH ₂ | Cl | Cl | H | CH ₃ | CH ₃ | bond | G1 | - |
| 7367 | CH ₂ | CF ₃ | OCH ₃ | H | H | CH ₃ | bond | G1 | - |
| 7368 | CH ₂ | CH ₃ | OCH ₃ | F | H | CH ₃ | bond | G1 | - |
| 7369 | O | Cl | Cl | H | H | C ₂ H ₅ | bond | G1 | - |
| 7370 | O | Cl | CF ₃ | H | H | C ₂ H ₅ | bond | G1 | - |
| 7371 | CH ₂ | Cl | OCF ₃ | H | H | C ₂ H ₅ | bond | G1 | - |
| 7372 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₂ H ₅ | bond | G1 | - |
| 7373 | CH ₂ | Cl | Cl | H | CH ₃ | C ₂ H ₅ | bond | G1 | - |
| 7374 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₂ H ₅ | bond | G1 | - |
| 7375 | CH ₂ | CH ₃ | OCH ₃ | F | H | C ₂ H ₅ | bond | G1 | - |
| 7376 | O | Cl | Cl | H | H | C ₃ H ₇ | bond | G1 | - |
| 7377 | O | Cl | CF ₃ | H | H | C ₃ H ₇ | bond | G1 | - |
| 7378 | CH ₂ | Cl | OCF ₃ | H | H | C ₃ H ₇ | bond | G1 | - |
| 7379 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | C ₃ H ₇ | bond | G1 | - |
| 7380 | CH ₂ | Cl | Cl | H | CH ₃ | C ₃ H ₇ | bond | G1 | - |
| 7381 | CH ₂ | CF ₃ | OCH ₃ | H | H | C ₃ H ₇ | bond | G1 | - |
| 7382 | CH ₂ | CH ₃ | OCH ₃ | F | H | C ₃ H ₇ | bond | G1 | - |
| 7383 | O | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G1 | - |
| 7384 | O | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G1 | - |
| 7385 | CH ₂ | Cl | OCF ₃ | H | H | c-C ₃ H ₅ | bond | G1 | - |
| 7386 | CH ₂ | CH ₃ | OCH ₃ | Cl | H | c-C ₃ H ₅ | bond | G1 | - |
| 7387 | CH ₂ | Cl | Cl | H | CH ₃ | c-C ₃ H ₅ | bond | G1 | - |
| 7388 | CH ₂ | CF ₃ | OCH ₃ | H | H | c-C ₃ H ₅ | bond | G1 | - |
| 7389 | CH ₂ | CH ₃ | OCH ₃ | F | H | c-C ₃ H ₅ | bond | G1 | - |
| 7390 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G14 | oil |
| 7391 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G14 | - |

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|------|-----------------|----|-----------------|---|-----------------|---|------|------------------|---------|
| 7391 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G15 | oil |
| 7392 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G15 | - |
| 7393 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G16 | 139-140 |
| 7394 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G16 | - |
| 7395 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G17 | - |
| 7396 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G17 | oil |
| 7397 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G18 | - |
| 7398 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G18 | oil |
| 7399 | CH ₂ | Cl | Cl | H | CH ₃ | CH ₃ | bond | G8 | oil |
| 7400 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G19 | - |
| 7401 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G19 | oil |
| 7402 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G20 | oil |
| 7403 | CH ₂ | Cl | CF ₃ | H | H | c-C ₃ H ₅ | bond | G20 | - |
| 7404 | CH ₂ | Cl | Cl | H | H | C ₄ H ₉ | bond | G1 | oil |
| 7405 | CH ₂ | Cl | Cl | H | H | C ₆ H ₅ | C=O | C ₆ H | oil |
| 5 | | | | | | | | | |
| 7406 | CH ₂ | Cl | Cl | H | H | C ₆ H ₅ | C=O | G21 | oil |
| 7407 | CH ₂ | Cl | Cl | H | H | C ₆ H ₅ | C=O | G22 | oil |
| 7408 | CH ₂ | Cl | Cl | H | H | 4-F- C ₆ H ₄ CH ₂ | C=O | CH ₃ | oil |
| 7409 | CH ₂ | Cl | Cl | H | H | c-C ₃ H ₅ | bond | G23 | oil |

Key:

(a) G groups:





(b) Where a compound is indicated as an "oil", spectral data is provided as follows:

5 Example 7056 spectral data: MS (ESI): m/e 363 ($M+2$), 361 (M^+ , 100%).

Example 7086 spectral data: TLC R_f 0.25 (30:70 ethyl acetate-hexane). 1H NMR (300 MHz, $CDCl_3$): δ 8.91 (1H, s), 7.72 (1H, d, J = 9.2 Hz), 6.90-6.84 (2H, m), 6.08 (1H, ddq, J = 15.4 Hz, 6.6H, 1.4 Hz), 5.67 (1H, dqd, J = 15.4 Hz, 6.5H, 1.5 Hz), 5.24 (1H, br pentet, J = 7.0 Hz), 3.85 (3H, s),
 10 2.96 (2H, dq, J = 7.5, 1.1 Hz), 2.47 (3H, s), 1.81 (3H, d, J = 7.0 Hz), 1.73 (3H, dt, J = 6.2, 1.3 Hz), 1.41 (3H, t, J = 7.5 Hz). MS (NH_3 -CI): m/e 339 (3), 338 (23), 337 (100).

Example 7116 spectral data: TLC R_f 0.15 (30:70 ethyl acetate-hexane). 1H NMR (300 MHz, $CDCl_3$): δ 8.96 (1H, s), 7.68 (1H, d, J = 8.4 Hz), 7.09 (1H, d, J = 2.6 Hz), 6.96 (1H, dd, J = 8.4, 2.6 Hz), 6.09 (1H, ddq, J = 15.4 Hz, 6.6H, 1.8 Hz), 5.67 (1H, dqd, J = 15.4 Hz, 6.5H, 1.4 Hz), 5.23 (1H, br pentet, J = 6.8 Hz), 3.87 (3H, s), 2.98 (2H, q, J = 7.5 Hz), 1.82
 15 (3H, d, J = 7.0 Hz), 1.73 (3H, dt, J = 6.6, 1.3 Hz), 1.40 (3H, t, J = 7.5 Hz). MS (NH_3 -CI): m/e 360 (7), 359 (33), 358 (23), 357 (100).

Example 7145 spectral data: m.p. 78-79 °C. TLC R_f 0.52 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.01 (1H, s), 7.86-7.81 (2H, m), 7.68 (1H, d, J = 8.0 Hz), 6.38 (2H, ddd, J = 17.2 Hz, 10.6 Hz, 5.8 Hz), 5.90-5.83 (1H, m), 5.40 (2H, dd, J = 10.6, 1.3 Hz), 5.29 (2H, dt, J = 17.2, 0.9 Hz), 2.97 (2H, q, J = 7.6 Hz), 1.41 (3H, t, J = 7.6 Hz). MS (NH₃-CI): m/e 396 (8), 395 (36), 394 (25), 393 (100). Analysis calculated for C₁₅H₁₆ClF₃N₄: C, 58.10; H, 4.12; N, 14.26; found: C, 58.14; H, 4.28; N, 13.74.

Example 7146 spectral data: TLC R_f 0.43 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.99 (1H, s), 7.84-7.79 (2H, m), 7.67 (1H, dd, J = 8.5, 1.1 Hz), 6.10 (1H, ddq, J = 15.4 Hz, 6.8 Hz, 1.8 Hz), 5.70 (1H, dqd, J = 15.4 Hz, 6.5 Hz, 1.1 Hz), 5.24 (1H, pentet, J = 7.0 Hz), 2.99 (2H, q, J = 7.5 Hz), 1.83 (3H, d, J = 7.0 Hz), 1.74 (3H, dt, J = 6.6, 1.3 Hz), 1.40 (3H, t, J = 7.5 Hz). MS (NH₃-CI): m/e 398 (7), 397 (36), 396 (25), 395 (100).

Example 7231 spectral data: m.p. 78-88 °C. TLC R_f 0.55 (50:50 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): Major isomer: δ 8.90 (1H, s), 6.95 (2H, s), 4.68-3.05 (6H, m), 3.02-2.92 (2H, m), 2.70-2.55 (2H, m), 2.32 (3H, s), 2.20-2.00 (2H, m), 2.05 (3H, s), 1.96 (3H, s), 1.70-1.45 (4H, m), 1.39 (3H, t, J = 7.7 Hz), 0.93 (3H, t, J = 7.3 Hz); Minor isomer: δ 8.89 (1H, s), 6.95 (2H, s), 4.68-3.05 (6H, m), 3.02-2.92 (2H, m), 2.70-2.55 (2H, m), 2.32 (3H, s), 2.20-2.00 (2H, m), 2.06 (3H, s), 2.01 (3H, s), 1.70-1.45 (4H, m), 1.38 (3H, t, J = 7.7 Hz), 0.90 (3H, t, J = 7.3 Hz). MS (NH₃-CI): m/e calc'd for C₂₅H₃₅N₄O₂: 423.2760, found 423.2748; 425 (5), 424 (29), 423 (100). Analysis calc'd for C₂₅H₃₄N₄O₂•H₂O: C, 68.15; H, 8.24; N, 12.72; found: C, 67.80; H, 7.89; N, 12.24.

Example 7234 spectral data: TLC R_f 0.46 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.99 (1H, s), 7.87 (1H, d, J = 8.0 Hz), 7.83 (1H, s), 7.68 (1H, d, J = 8.0 Hz), 6.50 (1H, d, J = 3.0 Hz), 5.99 (1H, d, J = 3.0 Hz), 5.10 (1H, d, J = 10.6 Hz), 2.99-2.79 (2H, m), 2.20 (3H, s), 2.10-2.00 (1H, m), 1.30 (3H, t, J = 7.5 Hz), 1.00-0.90 (1H, m), 0.71-0.59 (2H, m), 0.56-0.46 (1H, m). MS (NH₃-CI): m/e 463 (35), 461 (100).

Example 7241 spectral data: MS (NH₃-CI): m/e 371 (M+H⁺, 100%).

Example 7243 spectral data: TLC R_f 0.43 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.01 (1H, s), 7.85 (1H, d, J = 8.0 Hz), 7.83 (1H, s), 7.69 (1H, d, J = 8.0 Hz), 5.24 (1H, dd, J = 8.4, 2.5 Hz), 3.28 (1H, dq, J = 15.5, 7.5 Hz), 3.14 (1H, dq, J = 15.5, 7.5 Hz), 2.56 (1H, d, J = 2.5 Hz), 1.78-1.67 (1H, m), 1.48 (3H, t, J = 7.5 Hz), 0.92-0.81 (2H, m),

0.66-0.49 (2H, m). MS (NH₃-CI): *m/e* calculated for C₂₀H₁₇ClF₃N₄: 405.1094, found 405.1098; 408 (8), 407 (34), 406 (25), 405 (100).

Example 7249 spectral data: TLC R_f 0.19 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.93 (1H, s), 7.72 (1H, d, *J* = 8.5 Hz), 7.37 (1H, d, *J* = 2.5 Hz), 7.18 (1H, dd, *J* = 8.5, 2.5 Hz), 5.23 (1H, dd, *J* = 8.1, 2.6 Hz), 3.92 (3H, s), 3.31-3.04 (2H, m), 2.54 (1H, d, *J* = 2.6 Hz), 1.76-1.64 (1H, m), 1.47 (3H, t, *J* = 7.5 Hz), 0.90-0.80 (2H, m), 0.64-0.52 (2H, m). MS (NH₃-CI): *m/e* calc'd for C₂₁H₂₀F₃N₄O: 401.1603, found 401.1602; 403 (6), 402 (24), 401 (100).

Example 7250 spectral data: TLC R_f 0.17 (20:80 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.01 (1H, s), 7.67 (1H, d, *J* = 8.5 Hz), 7.58 (1H, d, *J* = 1.8 Hz), 7.41 (1H, dd, *J* = 8.5, 1.8 Hz), 5.53 (1H, dt, *J* = 8.0, 2.6 Hz), 3.20 (1H, dq, *J* = 15.8, 7.5 Hz), 3.05 (1H, dq, *J* = 15.8, 7.5 Hz), 2.55 (1H, d, *J* = 2.6 Hz), 2.42-2.29 (1H, m), 2.28-2.15 (1H, m), 1.46 (3H, t, *J* = 7.5 Hz), 1.04 (3H, t, *J* = 7.5 Hz). MS (NH₃-CI): *m/e* calc'd for C₁₈H₁₇Cl₂N₄: 359.0830, found 359.0835; 364 (2), 363 (12), 362 (14), 361 (67), 360 (24), 359 (100).

Example 7259 spectral data: TLC R_f 0.22 (20:80 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.01 (1H, s), 7.67 (1H, d, *J* = 8.1 Hz), 7.58 (1H, d, *J* = 1.8 Hz), 7.40 (1H, dd, *J* = 8.1, 1.8 Hz), 5.63 (1H, dt, *J* = 7.9, 2.5 Hz), 3.20 (1H, dq, *J* = 15.7, 7.7 Hz), 3.05 (1H, dq, *J* = 15.7, 7.7 Hz), 2.54 (1H, d, *J* = 2.5 Hz), 2.37-2.24 (1H, m), 2.19-2.06 (1H, m), 1.60-1.45 (1H, m), 1.46 (3H, t, *J* = 7.7 Hz), 1.39-1.25 (1H, m), 0.99 (3H, t, *J* = 7.3 Hz). MS (NH₃-CI): *m/e* calc'd for C₁₉H₁₉Cl₂N₄: 373.0987, found 373.0984; 378 (3), 377 (12), 376 (15), 375 (66), 374 (26), 373 (100).

Example 7261 spectral data: TLC R_f 0.52 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.03 (1H, s), 7.84 (2H, m), 7.68 (1H, dd, *J* = 7.3, 0.7 Hz), 5.65 (1H, dt, *J* = 8.1, 2.6 Hz), 3.24-3.02 (2H, m), 2.55 (1H, d, *J* = 2.6 Hz), 2.33-2.25 (1H, m), 2.20-2.12 (1H, m), 1.46 (3H, t, *J* = 7.5 Hz), 1.00 (3H, t, *J* = 7.3 Hz). MS (NH₃-CI): *m/e* calc'd for C₂₀H₁₉ClF₃N₄: 407.1250, found 407.1243; 410 (8), 409 (36), 408 (25), 407 (100).

Example 7266 spectral data: TLC R_f 0.19 (20:80 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.01 (1H, d, *J* = 1.5 Hz), 7.38 (1H, d, *J* = 1.8 Hz), 7.24 (1H, d, *J* = 1.8 Hz), 5.70-5.58 (1H, m), 3.24-3.00 (2H, m), 2.55 (1H, d, *J* = 2.5 Hz), 2.40-2.25 (1H, m), 2.20-2.05 (1H, m), 2.10 (3H, d, *J* = 1.8 Hz), 1.62-1.47 (1H, m), 1.43 (3H, t, *J* = 7.5 Hz), 1.42-

1.27 (1H, m), 1.00 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-Cl}$): m/e calc'd for $\text{C}_{20}\text{H}_{21}\text{Cl}_2\text{N}_4$: 387.1143, found 387.1144; 392 (3), 391 (12), 390 (16), 389 (66), 388 (27), 387 (100).

Example 7268 spectral data: TLC R_f 0.29 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 9.01 (1H, s), 7.67 (1H, d, $J = 8.5$ Hz), 7.58 (1H, d, $J = 2.2$ Hz), 7.41 (1H, dd, $J = 8.5, 2.2$ Hz), 5.60 (1H, dt, $J = 7.9, 2.6$ Hz), 3.19 (1H, dq, $J = 15.3, 7.3$ Hz), 3.05 (1H, dq, $J = 15.3, 7.3$ Hz), 2.54 (1H, d, $J = 2.6$ Hz), 2.38-2.23 (1H, m), 2.20-2.05 (1H, m), 1.58-1.44 (1H, m), 1.46 (3H, t, $J = 7.3$ Hz), 1.40-1.23 (5H, m), 0.87 (3H, t, $J = 7.0$ Hz). MS ($\text{NH}_3\text{-Cl}$): m/e calc'd for $\text{C}_{21}\text{H}_{23}\text{Cl}_2\text{N}_4$: 401.1300, found 401.1300; 406 (3), 405 (13), 404 (17), 403 (69), 402 (28), 401 (100).

Example 7270 spectral data: TLC R_f 0.60 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 9.03 (1H, s), 7.84 (2H, m), 7.68 (1H, dd, $J = 9.1, 0.7$ Hz), 5.62 (1H, dt, $J = 8.1, 2.6$ Hz), 3.24-3.02 (2H, m), 2.55 (1H, d, $J = 2.6$ Hz), 2.34-2.27 (1H, m), 2.19-2.13 (1H, m), 1.46 (3H, t, $J = 7.3$ Hz), 1.40-1.25 (6H, m), 0.88 (3H, t, $J = 7.0$ Hz). MS ($\text{NH}_3\text{-Cl}$): m/e calc'd for $\text{C}_{22}\text{H}_{23}\text{ClF}_3\text{N}_4$: 435.1563, found 435.1566; 438 (9), 437 (36), 436 (27), 435 (100).

Example 7279 spectral data: TLC R_f 0.31 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.97 (1H, s), 7.84 (2H, m), 7.68 (1H, d, $J = 7.7$ Hz), 4.74-4.67 (1H, m), 3.45-3.36 (1H, m), 3.03 (2H, q, $J = 7.7$ Hz), 3.00-2.93 (1H, m), 1.93 (1H, t, $J = 2.7$ Hz), 1.86 (3H, d, $J = 7.0$ Hz), 1.43 (3H, t, $J = 7.5$ Hz). MS ($\text{NH}_3\text{-Cl}$): m/e 396 (7), 395 (34), 394 (24), 393 (100).

Example 7286 spectral data: TLC R_f 0.29 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.97 (1H, s), 7.68 (1H, d, $J = 8.4$ Hz), 7.58 (1H, d, $J = 1.8$ Hz), 7.41 (1H, dd, $J = 8.4, 1.8$ Hz), 5.19 (1H, dq, $J = 8.4, 2.6$ Hz), 3.26 (1H, dq, $J = 15.7, 7.3$ Hz), 3.14 (1H, dq, $J = 15.7, 7.3$ Hz), 1.88 (3H, d, $J = 2.6$ Hz), 1.70-1.60 (1H, m), 1.47 (3H, t, $J = 7.3$ Hz), 0.89-0.78 (2H, m), 0.60-0.43 (2H, m). MS ($\text{NH}_3\text{-Cl}$): m/e calc'd for $\text{C}_{20}\text{H}_{19}\text{Cl}_2\text{N}_4$: 385.0986, found 385.0992; 390 (3), 389 (12), 388 (15), 387 (66), 386 (26), 385 (100).

Example 7288 spectral data: MS ($\text{NH}_3\text{-Cl}$): m/e 419 ($\text{M}+\text{H}^+$, 100%).

Example 7295 spectral data: TLC R_f 0.19 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.99 (1H, s), 7.67 (1H, d, $J = 8.4$ Hz), 7.57 (1H, d, $J = 2.2$ Hz), 7.40 (1H, dd, $J = 8.4, 2.2$ Hz), 5.49 (1H, tq, $J = 7.7, 2.2$ Hz), 3.19 (1H, dq, $J = 15.3, 7.7$ Hz), 3.05 (1H, dq, $J = 15.3, 7.7$

Hz), 2.26 (1H, dq, J = 21.3, 7.7 Hz), 2.13 (1H, dq, J = 21.3, 7.7 Hz), 1.87 (3H, d, J = 2.2 Hz), 1.45 (3H, t, J = 7.7 Hz), 1.01 (3H, t, J = 7.7 Hz). MS (NH₃-CI): m/e calc'd for C₁₉H₁₉Cl₂N₄: 373.0987, found 373.0987; 378 (3), 377 (13), 376 (15), 375 (68), 374 (25), 373 (100).

- 5 Example 7297 spectral data: TLC R_f 0.48 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.01 (1H, s), 7.83 (2H, m), 7.67 (1H, dd, J = 7.4, 0.8 Hz), 5.51 (1H, dt, J = 8.1, 2.2 Hz), 3.25-3.03 (2H, m), 2.35-2.13 (2H, m), 1.88 (3H, d, J = 2.2 Hz), 1.45 (3H, t, J = 7.5 Hz), 1.01 (3H, t, J = 7.3 Hz). MS (NH₃-CI): m/e calc'd for C₂₀H₁₉ClF₃N₄: 407.1250, found 407.1267; 410 (8), 409 (35), 408 (25), 407 (100).

Example 7306 spectral data: MS (NH₃-CI): m/e 421 (M+H⁺, 100%).

- Example 7324 spectral data: TLC R_f 0.38 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.99 (1H, s), 7.84 (1H, d, J = 8.4 Hz), 7.83 (1H, d, J = 1.8 Hz), 7.68 (1H, dd, J = 8.4, 1.8 Hz), 7.36 (1H, d, J = 3 Hz), 15 6.51 (1H, d, J = 5 Hz), 6.39 (1H, dd, J = 5, 3 Hz), 5.78 (1H, dd, J = 9, 7 Hz), 3.00-2.85 (2H, m), 2.75-2.52 (2H, m), 1.37 (3H, t, J = 7.5 Hz), 0.98 (3H, t, J = 7.5 Hz). MS (NH₃-CI): m/e 439 (1), 438 (8), 437 (34), 436 (26), 435 (100).

- Example 7349 spectral data: TLC R_f 0.20 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 9.00 (1H, s), 7.87 (1H, d, J = 8.0 Hz), 7.83 (1H, s), 7.69 (1H, d, J = 8.0 Hz), 5.01 (1H, d, J = 10.6 Hz), 2.93 (1H, dq, J = 15.9, 7.5 Hz), 2.75 (1H, dq, J = 15.9, 7.5 Hz), 2.58 (3H, s), 2.04-1.94 (1H, m), 1.93 (3H, s), 1.33 (3H, t, J = 7.5 Hz), 1.32-1.22 (1H, m), 1.00-0.87 (1H, m), 0.74-0.60 (3H, m). MS (NH₃-CI): m/e calculated for 20 C₂₃H₂₂ClF₃N₅O: 476.1465, found 476.1469; 478 (35), 476 (100).

- Example 7351 spectral data: TLC R_f 0.44 (30:70 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.99 (1H, s), 7.88-7.82 (2H, m), 7.68 (1H, d, J = 8.0 Hz), 6.35 (1H, ddd, J = 17.2 Hz, 10.6 Hz, 5.1 Hz), 5.33 (1H, br d, J = 10.6 Hz), 5.26 (1H, br d, J = 17.2 Hz), 4.43-4.37 (1H, m), 3.02-2.90 30 (2H, m), 1.99-1.89 (1H, m), 1.41 (3H, t, J = 7.5 Hz), 0.94-0.84 (1H, m), 0.62-0.52 (2H, m), 0.40-0.30 (1H, m). MS (NH₃-CI): m/e 411 (1), 410 (7), 409 (34), 408 (25), 407 (100).

- Example 7352 spectral data: TLC R_f 0.13 (20:80 ethyl acetate-hexane). ¹H NMR (300 MHz, CDCl₃): δ 8.96 (1H, s), 7.69 (1H, d, J = 8.4 Hz), 7.58 (1H, d, J = 2.2 Hz), 7.41 (1H, dd, J = 8.8, 2.2 Hz), 6.33 (1H, ddd, J = 17.2, 10.6, 5.2 Hz), 5.35-5.20 (2H, m), 4.42-4.35 (1H, m), 3.03-2.88 (2H, m), 2.00-1.89 (1H, m), 1.40 (3H, t, J = 7.6 Hz), 0.92-0.82 (1H, m), 0.62-0.52 (2H, m), 0.40-0.30 (1H, m). MS (NH₃-CI): m/e calc'd for C₁₉H₁₉Cl₂N₄: 35

- 373.1000, found 373.0995; 378 (3), 377 (12), 376 (15), 375 (66), 374 (26), 373 (100).
- Example 7355 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 337 ($\text{M}+\text{H}^+$, 100%).
- Example 7356 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 365 ($\text{M}+\text{H}^+$, 100%).
- 5 Example 7357 spectral data: TLC R_f 0.19 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.91 (1H, s), 7.70 (1H, d, $J = 8.4$ Hz), 7.35 (1H, d, $J = 2.6$ Hz), 7.19 (1H, dd, $J = 8.4, 2.6$ Hz), 6.42 (1H, ddd, $J = 16.9, 10.3, 6.6$ Hz), 5.27 (1H, d, $J = 10.2$ Hz), 5.14 (1H, d, $J = 17.3$ Hz), 5.08-4.99 (1H, m), 3.91 (3H, s), 2.99-2.90 (2H, m), 2.42-2.29 (1H, m),
- 10 2.27-2.15 (1H, m), 1.39 (3H, t, $J = 7.5$ Hz), 1.38-1.10 (2H, m), 0.95 (3H, t, $J = 7.1$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{21}\text{H}_{23}\text{F}_3\text{N}_4\text{O}$: 405.1915, found 405.1923; 407 (5), 406 (24), 405 (100). Analysis calc'd for $\text{C}_{21}\text{H}_{23}\text{F}_3\text{N}_4\text{O}$: C, 62.37; H, 5.73; N, 13.85; found: C, 62.42; H, 5.73; N, 13.48.
- 15 Example 7358 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 379 ($\text{M}+\text{H}^+$, 100%).
- Example 7360 spectral data: TLC R_f 0.13 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.91 (1H, s), 7.68 (1H, d, $J = 8.8$ Hz), 7.35 (1H, d, $J = 2.6$ Hz), 7.16 (1H, dd, $J = 8.8, 2.6$ Hz), 6.15-6.05 (1H, m), 5.73-5.63 (1H, m), 5.28-5.18 (1H, m), 3.91 (3H, s), 2.96 (2H, q, $J = 7.4$ Hz),
- 20 1.82 (3H, d, $J = 7.3$ Hz), 1.74 (3H, dt, $J = 6.6, 1.3$ Hz), 1.39 (3H, t, $J = 7.4$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{20}\text{H}_{22}\text{F}_3\text{N}_4\text{O}$: 391.1733, found 391.1736; 393 (3), 392 (23), 391 (100).
- Example 7361 spectral data: TLC R_f 0.43 (50:50 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.96 (1H, s), 7.42 (1H, s), 6.84 (1H, s), 5.55
- 25 (1H, dt, $J = 5.5, 2.2$ Hz), 3.94 (3H, s), 3.92 (3H, s), 3.49-2.98 (2H, m), 2.54 (1H, d, $J = 2.6$ Hz), 2.45 (3H, s), 2.35-2.16 (2H, m), 1.48 (3H, t, $J = 7.5$ Hz), 1.03 (3H, t, $J = 7.5$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{21}\text{H}_{23}\text{N}_4\text{O}_2$: 365.1978, found 365.1966; 367 (6), 366 (24), 365 (100).
- Example 7390 spectral data: TLC R_f 0.45 (30:70 ethyl acetate-hexane). ^1H
- 30 NMR (300 MHz, CDCl_3): δ 8.99 (1H, s), 7.88 (1H, d, $J = 8.0$ Hz), 7.83 (1H, s), 7.69 (1H, d, $J = 8.0$ Hz), 7.30-7.22 (1H, m), 7.07-7.01 (1H, m), 6.99-6.92 (1H, m), 5.25 (1H, d, $J = 10.2$ Hz), 2.97-2.78 (2H, m), 2.23 (1H, br), 1.32 (3H, t, $J = 7.3$ Hz), 1.10-1.00 (1H, m), 0.81-0.71 (1H, m), 0.64-0.54 (1H, m), 0.50-0.40 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for
- 35 $\text{C}_{22}\text{H}_{19}\text{ClF}_3\text{N}_4\text{S}$: 463.0971, found 463.0960; 467 (3), 466 (10), 465 (99), 464 (28), 463 (100).
- Example 7392 spectral data: TLC R_f 0.44 (30:70 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.99 (1H, s), 7.88 (1H, d, $J = 8.0$ Hz), 7.83 (1H,

s), 7.68 (1H, d, $J = 8.0$ Hz), 7.30 (1H, br d, $J = 4.8$ Hz), 7.18 (1H, br d, $J = 4.8$ Hz), 6.92 (1H, m), 5.12 (1H, d, $J = 9.9$ Hz), 2.92-2.67 (2H, m), 2.13 (1H, br), 1.28 (3H, t, $J = 7.5$ Hz), 1.08-0.99 (1H, m), 0.79-0.69 (1H, m), 0.55-0.45 (2H, m). MS ($\text{NH}_3\text{-CI}$): m/e calculated for $\text{C}_{22}\text{H}_{19}\text{ClF}_3\text{N}_4\text{S}$: 463.0971, found 463.0953; 467 (3), 466 (10), 465 (39), 464 (29), 463 (100).

Example 7396 spectral data: TLC R_f 0.27 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.96 (1H, s), 7.67 (1H, d, $J = 8.1$ Hz), 7.58 (1H, d, $J = 1.8$ Hz), 7.41 (1H, dd, $J = 8.1, 1.8$ Hz), 6.86 (1H, s), 5.83 (1H, dd, $J = 9.9, 6.2$ Hz), 4.43 (2H, q, $J = 7.3$ Hz), 2.98 (2H, q, $J = 7.7$ Hz), 2.91-2.78 (1H, m), 2.63-2.49 (1H, m), 1.42 (3H, t, $J = 7.7$ Hz), 1.40 (3H, t, $J = 7.3$ Hz), 1.39-1.19 (2H, m), 1.00 (3H, t, $J = 7.3$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{23}\text{H}_{24}\text{Cl}_2\text{N}_5\text{O}_3$: 488.1256, found 488.1252; 493 (3), 492 (13), 491 (18), 490 (68), 489 (28), 488 (100).

Example 7398 spectral data: TLC R_f 0.11 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.99 (1H, s), 7.72 (1H, d, $J = 8.1$ Hz), 7.59 (1H, d, $J = 1.8$ Hz), 7.42 (1H, dd, $J = 8.1, 1.8$ Hz), 5.40 (1H, dd, $J = 10.4, 5.0$ Hz), 4.42 (2H, q, $J = 7.4$ Hz), 3.00-2.90 (2H, m), 2.66-2.52 (1H, m), 2.51-2.38 (1H, m), 1.46 (3H, t, $J = 7.4$ Hz), 1.41 (3H, t, $J = 7.3$ Hz), 1.40-1.10 (2H, m), 0.98 (3H, t, $J = 7.2$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{24}\text{H}_{25}\text{Cl}_2\text{N}_6\text{O}_4$: 531.1315, found 531.1315; 531 (100).

Example 7399 spectral data: TLC R_f 0.13 (20:80 ethyl acetate-hexane). ^1H NMR (300 MHz, CDCl_3): δ 8.98 (1H, s), 7.38 (1H, d, $J = 1.8$ Hz), 7.23 (1H, d, $J = 1.8$ Hz), 6.15-6.06 (1H, m), 5.76-5.63 (1H, m), 5.26-5.20 (1H, m), 2.96 (2H, q, $J = 7.4$ Hz), 2.10 (3H, s), 1.83 (3H, d, $J = 7.0$ Hz), 1.74 (3H, d, $J = 6.6$ Hz), 1.37 (3H, t, $J = 7.4$ Hz). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{19}\text{H}_{21}\text{Cl}_2\text{N}_4$: 375.1117, found 375.1123; 380 (2), 379 (12), 378 (15), 377 (66), 376 (26), 375 (100).

Example 7401 spectral data: TLC R_f 0.20 (ethyl acetate). ^1H NMR (300 MHz, CDCl_3): δ 8.99 (1H, s), 7.71 (1H, d, $J = 8.4$ Hz), 7.58 (1H, d, $J = 1.8$ Hz), 7.41 (1H, dd, $J = 8.4, 1.8$ Hz), 7.11 (1H, d, $J = 1.1$ Hz), 6.87 (1H, d, $J = 1.1$ Hz), 5.41 (1H, d, $J = 10.3$ Hz), 3.34 (3H, s), 3.08 (1H, dq, $J = 15.8, 7.7$ Hz), 2.89 (1H, dq, $J = 15.8, 7.7$ Hz), 2.39-2.25 (1H, m), 1.14 (3H, t, $J = 7.7$ Hz), 1.07-0.97 (1H, m), 0.70-0.58 (2H, m), 0.52-0.42 (1H, m). MS ($\text{NH}_3\text{-CI}$): m/e calc'd for $\text{C}_{21}\text{H}_{21}\text{Cl}_2\text{N}_6$: 427.1205, found 427.1196; 429 (66), 427 (100).

Example 7402 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 424 ($\text{M}+\text{H}^+$, 100%).

Example 7404 spectral data: MS ($\text{NH}_3\text{-CI}$): m/e 419 ($\text{M}+\text{H}^+$, 100%).

- Example 7405 spectral data: MS (NH₃-CI): m/e 487 (M+H⁺, 100%).
Example 7406 spectral data: MS (NH₃-CI): m/e 501 (M+H⁺, 100%).
Example 7407 spectral data: MS (NH₃-CI): m/e 517 (M+H⁺, 100%).
Example 7408 spectral data: MS (NH₃-CI): m/e 457 (M+H⁺, 100%).
5 Example 7409 spectral data: MS (NH₃-CI): m/e 429 (M+H⁺, 100%).

Utility

10

CRF-R1 Receptor Binding Assay for the Evaluation of Biological Activity

The following is a description of the isolation of cell
15 membranes containing cloned human CRF-R1 receptors for use in
the standard binding assay as well as a description of the
assay itself.

Messenger RNA was isolated from human hippocampus. The
mRNA was reverse transcribed using oligo (dt) 12-18 and the
20 coding region was amplified by PCR from start to stop codons.
The resulting PCR fragment was cloned into the EcoRV site of
pGEMV, from whence the insert was reclaimed using XhoI + XbaI
and cloned into the XhoI + XbaI sites of vector pm3ar (which
contains a CMV promoter, the SV40 't' splice and early poly A
25 signals, an Epstein-Barr viral origin of replication, and a
hygromycin selectable marker). The resulting expression
vector, called phchCRFR was transfected in 293EBNA cells and
cells retaining the episome were selected in the presence of
400 mM hygromycin. Cells surviving 4 weeks of selection in
30 hygromycin were pooled, adapted to growth in suspension and
used to generate membranes for the binding assay described
below. Individual aliquots containing approximately 1×10^8
of the suspended cells were then centrifuged to form a pellet
and frozen.

35 For the binding assay a frozen pellet described above
containing 293EBNA cells transfected with hCRFR1 receptors is
homogenized in 10 mL of ice cold tissue buffer (50 mM HEPES
buffer pH 7.0, containing 10 mM MgCl₂, 2 mM EGTA, 1 mg/L

aprotinin, 1 mg/mL leupeptin and 1 mg/mL pepstatin). The homogenate is centrifuged at 40,000 x g for 12 min and the resulting pellet rehomogenized in 10 mL of tissue buffer. After another centrifugation at 40,000 x g for 12 min, the
5 pellet is resuspended to a protein concentration of 360 mg/mL to be used in the assay.

Binding assays are performed in 96 well plates; each well having a 300 mL capacity. To each well is added 50 mL of test drug dilutions (final concentration of drugs range from 10^{-10}
10 to 10^{-5} M), 100 mL of ^{125}I -ovine-CRF (^{125}I -o-CRF) (final concentration 150 pM) and 150 mL of the cell homogenate described above. Plates are then allowed to incubate at room temperature for 2 hours before filtering the incubate over GF/F filters (presoaked with 0.3% polyethyleneimine) using an
15 appropriate cell harvester. Filters are rinsed 2 times with ice cold assay buffer before removing individual filters and assessing them for radioactivity on a gamma counter.

Curves of the inhibition of ^{125}I -o-CRF binding to cell membranes at various dilutions of test drug are analyzed by:
20 the iterative curve fitting program LIGAND [P.J. Munson and D. Rodbard, *Anal. Biochem.* 107:220 (1980), which provides K_i values for inhibition which are then used to assess biological activity.

Alternatively, tissues and cells which naturally express
25 CRF receptors can be employed in binding assays analogous to those described above.

A compound is considered to be active if it has a K_i value of less than about 10000 nM for the inhibition of CRF.

30

Inhibition of CRF-Stimulated Adenylate Cyclase Activity

Inhibition of CRF-stimulated adenylate cyclase activity can be performed as described by G. Battaglia et al. *Synapse* 1:572 (1987). Briefly, assays are carried out
35 at 37 °C for 10 min in 200 mL of buffer containing 100 mM Tris-HCl (pH 7.4 at 37 °C), 10 mM MgCl_2 , 0.4 mM EGTA, 0.1% BSA, 1 mM isobutylmethylxanthine (IBMX), 250 units/mL phosphocreatine kinase, 5 mM creatine phosphate, 100 mM

guanosine 5'-triphosphate, 100 nM oCRF, antagonist peptides (concentration range 10^{-9} to 10^{-6} M) and 0.8 mg original wet weight tissue (approximately 40-60 mg protein). Reactions are initiated by the addition of 1 mM ATP/ 32 P]ATP
5 (approximately 2-4 mCi/tube) and terminated by the addition of 100 μ L of 50 mM Tris-HCL, 45 mM ATP and 2% sodium dodecyl sulfate. In order to monitor the recovery of cAMP, 1 μ L of [3 H]cAMP (approximately 40,000 dpm) is added to each tube prior to separation. The separation of [32 P]cAMP from
10 [32 P]ATP is performed by sequential elution over Dowex and alumina columns.

In vivo Biological Assay

The *in vivo* activity of the compounds of the present
15 invention can be assessed using any one of the biological assays available and accepted within the art. Illustrative of these tests include the Acoustic Startle Assay, the Stair Climbing Test, and the Chronic Administration Assay. These and other models useful for the testing of compounds
20 of the present invention have been outlined in C.W. Berridge and A.J. Dunn *Brain Research Reviews* 15:71 (1990). Compounds may be tested in any species of rodent or small mammal.

25 Compounds of this invention have utility in the treatment of imbalances associated with abnormal levels of corticotropin releasing factor in patients suffering from depression, affective disorders, and/or anxiety.

Compounds of this invention can be administered to
30 treat these abnormalities by means that produce contact of the active agent with the agent's site of action in the body of a mammal. The compounds can be administered by any conventional means available for use in conjunction with pharmaceuticals either as individual therapeutic agent or
35 in combination of therapeutic agents. They can be administered alone, but will generally be administered with a pharmaceutical carrier selected on the basis of the

chosen route of administration and standard pharmaceutical practice.

The dosage administered will vary depending on the use and known factors such as pharmacodynamic character of the particular agent, and its mode and route of administration; the recipient's age, weight, and health; nature and extent of symptoms; kind of concurrent treatment; frequency of treatment; and desired effect. For use in the treatment of said diseases or conditions, the compounds of this invention can be orally administered daily at a dosage of the active ingredient of 0.002 to 200 mg/kg of body weight. Ordinarily, a dose of 0.01 to 10 mg/kg in divided doses one to four times a day, or in sustained release formulation will be effective in obtaining the desired pharmacological effect.

Dosage forms (compositions) suitable for administration contain from about 1 mg to about 100 mg of active ingredient per unit. In these pharmaceutical compositions, the active ingredient will ordinarily be present in an amount of about 0.5 to 95% by weight based on the total weight of the composition.

The active ingredient can be administered orally is solid dosage forms, such as capsules, tablets and powders; or in liquid forms such as elixirs, syrups, and/or suspensions. The compounds of this invention can also be administered parenterally in sterile liquid dose formulations.

Gelatin capsules can be used to contain the active ingredient and a suitable carrier such as but not limited to lactose, starch, magnesium stearate, steric acid, or cellulose derivatives. Similar diluents can be used to make compressed tablets. Both tablets and capsules can be manufactured as sustained release products to provide for continuous release of medication over a period of time. Compressed tablets can be sugar-coated or film-coated to mask any unpleasant taste, or used to protect the active ingredients from the atmosphere, or to allow selective disintegration of the tablet in the gastrointestinal tract.

Liquid dose forms for oral administration can contain coloring or flavoring agents to increase patient acceptance.

In general, water, pharmaceutically acceptable oils, saline, aqueous dextrose (glucose), and related sugar solutions and glycols, such as propylene glycol or polyethylene glycol, are suitable carriers for parenteral solutions. Solutions for parenteral administration preferably contain a water soluble salt of the active ingredient, suitable stabilizing agents, and if necessary, buffer substances. Antioxidizing agents, such as sodium bisulfite, sodium sulfite, or ascorbic acid, either alone or in combination, are suitable stabilizing agents. Also used are citric acid and its salts, and EDTA. In addition, parenteral solutions can contain preservatives such as benzalkonium chloride, methyl- or propyl-paraben, and chlorobutanol.

Suitable pharmaceutical carriers are described in "Remington's Pharmaceutical Sciences", A. Osol, a standard
20 reference in the field.

Useful pharmaceutical dosage-forms for administration of the compounds of this invention can be illustrated as follows:

Capsules

A large number of units capsules are prepared by filling standard two-piece hard gelatin capsules each with 100 mg of powdered active ingredient, 150 mg lactose, 50 mg cellulose, and 6 mg magnesium stearate.

Soft Gelatin Capsules

A mixture of active ingredient in a digestible oil such as soybean, cottonseed oil, or olive oil is prepared and injected by means of a positive displacement was pumped
35 into gelatin to form soft gelatin capsules containing 100 mg of the active ingredient. The capsules were washed and dried.

Tablets

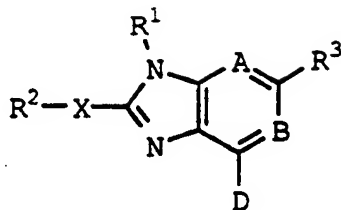
A large number of tablets are prepared by conventional procedures so that the dosage unit was 100 mg active ingredient, 0.2 mg of colloidal silicon dioxide, 5 mg of magnesium stearate, 275 mg of microcrystalline cellulose, 11 mg of starch, and 98.8 mg lactose. Appropriate coatings may be applied to increase palatability or delayed adsorption.

10 The compounds of this invention may also be used as reagents or standards in the biochemical study of neurological function, dysfunction, and disease.

15 Although the present invention has been described and exemplified in terms of certain preferred embodiments, other embodiments will be apparent to those skilled in the art. The invention is, therefore, not limited to the particular embodiments described and exemplified, but is capable of modification or variation without departing from
20 the spirit of the invention, the full scope of which is delineated by the appended claims.

WHAT IS CLAIMED IS:

1. A compound of formula (I)



5

(I)

or a stereoisomer or pharmaceutically acceptable salt form thereof, wherein:

10 A is N or C-R⁷;

B is N or C-R⁸;

provided that at least one of the groups A and B is N;

15

D is an aryl or heteroaryl group attached through an unsaturated carbon atom;

20

X is selected from the group CH-R⁹, N-R¹⁰, O, S(O)_n and a bond;

n is 0, 1 or 2;

25

R¹ is selected from the group C₁₋₁₀ alkyl, C₂₋₁₀ alkenyl, C₂₋₁₀ alkynyl, C₃₋₈ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, -SO₂-C₁₋₁₀ alkyl, -SO₂-R^{1a}, and -SO₂-R^{1b};

30

R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b}, -CONR^{13a}R^{16a}, 1-morpholinyl, 1-piperidinyl, 1-piperazinyl, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group

selected from the group -O-, -S(O)_n-, -NR^{13a}-,
-NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-, and wherein N₄ in
1-piperazinyl is substituted with 0-1 substituents
selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and
5 SO₂R^{14b};

R¹ is also substituted with 0-3 substituents independently
selected at each occurrence from the group R^{1a}, R^{1b},
R^{1c}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F,
10 I, C₁₋₄ haloalkyl, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₄ alkoxy-C₁₋₄
alkyl, and C₃₋₈ cycloalkyl which is substituted with 0-
1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is
replaced by -O-;

15 provided that R¹ is other than:

- (a) a cyclohexyl-(CH₂)₂- group;
- (b) a 3-cyclopropyl-3-methoxypropyl group;
- (c) an unsubstituted-(alkoxy)methyl group; and,
- (d) a 1-hydroxyalkyl group;

20

also provided that when R¹ alkyl substituted with OH, then
the carbon adjacent to the ring N is other than CH₂;

R^{1a} is aryl and is selected from the group phenyl, naphthyl,
25 indanyl and indenyl, each R^{1a} being substituted with
0-1 -OR¹⁷ and 0-5 substituents independently selected
at each occurrence from the group C₁₋₆ alkyl, C₃₋₆
cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro,
SH, -S(O)_nR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷,
30 -N(COR¹⁷)₂, -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a},
and -CONR^{17a}R^{19a};

R^{1b} is heteroaryl and is selected from the group pyridyl,
pyrimidinyl, triazinyl, furanyl, quinolinyl,
35 isoquinolinyl, thienyl, imidazolyl, thiazolyl,
indolyl, pyrrolyl, oxazolyl, benzofuranyl,
benzothienyl, benzothiazolyl, benzoxazolyl,

isoxazolyl, pyrazolyl, triazolyl, tetrazolyl,
indazolyl, 2,3-dihydrobenzofuranyl,
2,3-dihydrobenzothienyl,
2,3-dihydrobenzothienyl-S-oxide,
5 2,3-dihydrobenzothienyl-S-dioxide, indoliny, l,
benzoxazolin-2-onyl, benzodioxolanyl and benzodioxane,
each heteroaryl being substituted on 0-4 carbon atoms
with a substituent independently selected at each
occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl,
10 Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH,
-S(O)_mR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂,
-NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and
-CONR^{17a}R^{19a} and each heteroaryl being substituted on
any nitrogen atom with 0-1 substituents selected from
15 the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

R^{1c} is heterocyclyl and is a saturated or partially
saturated heteroaryl, each heterocyclyl being
substituted on 0-4 carbon atoms with a substituent
20 independently selected at each occurrence from the
group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄
haloalkyl, -CN, nitro, -OR^{13a}, SH, -S(O)_nR^{14b}, -COR^{13a},
-OC(O)R^{14b}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a},
-NR^{15a}CO₂R^{14b}, -NR^{13a}R^{16a}, and -CONR^{13a}R^{16a} and each
25 heterocyclyl being substituted on any nitrogen atom
with 0-1 substituents selected from the group R^{13a},
CO₂R^{14b}, COR^{14b} and SO₂R^{14b} and wherein any sulfur atom
is optionally monooxidized or dioxidized;

30 provided that R¹ is other than a -(CH₂)₁₋₄-aryl,
-(CH₂)₁₋₄-heteroaryl, or -(CH₂)₁₋₄-heterocycle, wherein
the aryl, heteroaryl, or heterocycle group is
substituted or unsubstituted;

35 R² is selected from the group C₁₋₄ alkyl, C₃₋₈ cycloalkyl,
C₂₋₄ alkenyl, and C₂₋₄ alkynyl and is substituted with

0-3 substituents selected from the group -CN, hydroxy, halo and C₁₋₄ alkoxy;

5 alternatively R², in the case where X is a bond, is selected from the group -CN, CF₃ and C₂F₅;

R³, R⁷ and R⁸ are independently selected at each occurrence from the group H, Br, Cl, F, I, -CN, C₁₋₄ alkyl, C₃₋₈ cycloalkyl, C₁₋₄ alkoxy, C₁₋₄ alkylthio, C₁₋₄ alkylsulfinyl, C₁₋₄ alkylsulfonyl, amino, C₁₋₄ alkylamino, (C₁₋₄ alkyl)₂amino and phenyl, each phenyl is substituted with 0-3 groups selected from the group C₁₋₇ alkyl, C₃₋₈ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, C₁₋₄ alkylthio, C₁₋₄ alkyl sulfinyl, C₁₋₄ alkylsulfonyl, C₁₋₆ alkylamino and (C₁₋₄ alkyl)₂amino;

20 provided that when R¹ is unsubstituted C₁₋₁₀ alkyl, then R³ is other than substituted or unsubstituted phenyl;

R⁹ and R¹⁰ are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₆ cycloalkyl-C₁₋₄ alkyl and C₃₋₈ cycloalkyl;

25 R¹³ is selected from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)-;

30 R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

35 R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)- and benzyl, each

benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy C₁₋₄ haloalkoxy, and dimethylamino;

5

R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

10

R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

15

R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

20

25

R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

R¹⁷ is selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₁₋₄ haloalkyl, R¹⁴S(O)_n-C₁₋₄ alkyl, and R^{17b}R^{19b}N-C₂₋₄ alkyl;

30

R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;

35

alternatively, in an $\text{NR}^{17}\text{R}^{19}$ moiety, R^{17} and R^{19} taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N_4 in
5 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13} , CO_2R^{14} , COR^{14} and SO_2R^{14} ;

alternatively, in an $\text{NR}^{17b}\text{R}^{19b}$ moiety, R^{17b} and R^{19b} taken together form 1-pyrrolidinyl, 1-morpholinyl,
10 1-piperidinyl or 1-piperazinyl, wherein N_4 in 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13} , CO_2R^{14} , COR^{14} and SO_2R^{14} ;

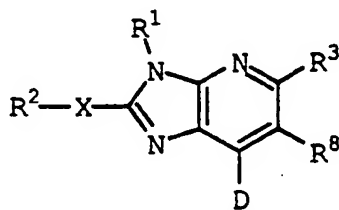
R^{17a} and R^{19a} are independently selected at each occurrence
15 from the group H, C_{1-6} alkyl, C_{3-10} cycloalkyl, C_{3-6} cycloalkyl- C_{1-6} alkyl and C_{1-4} haloalkyl;

aryl is independently selected at each occurrence from the group phenyl, naphthyl, indanyl and indenyl, each aryl
20 being substituted with 0-5 substituents independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, methylenedioxy, C_{1-4} alkoxy- C_{1-4} alkoxy, $-\text{OR}^{17}$, Br, Cl, F, I, C_{1-4} haloalkyl, $-\text{CN}$, $-\text{NO}_2$, SH, $-\text{S}(\text{O})_n\text{R}^{18}$, $-\text{COR}^{17}$, $-\text{CO}_2\text{R}^{17}$, $-\text{OC}(\text{O})\text{R}^{18}$, $-\text{NR}^{15}\text{COR}^{17}$,
25 $-\text{N}(\text{COR}^{17})_2$, $-\text{NR}^{15}\text{CONR}^{17}\text{R}^{19}$, $-\text{NR}^{15}\text{CO}_2\text{R}^{18}$, $-\text{NR}^{17}\text{R}^{19}$, and $-\text{CONR}^{17}\text{R}^{19}$ and up to 1 phenyl, each phenyl substituent being substituted with 0-4 substituents selected from the group C_{1-3} alkyl, C_{1-3} alkoxy, Br, Cl, F, I, $-\text{CN}$, dimethylamino, CF_3 , C_2F_5 , OCF_3 , SO_2Me and acetyl;

30 heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl,
35 isoxazolyl, triazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl,

- 2,3-dihydrobenzothienyl-S-oxide,
 2,3-dihydrobenzothienyl-S-dioxide, indolinyl,
 benzoxazolin-2-on-yl, benzodioxolanyl and
 benzodioxane, each heteroaryl being substituted 0-4
 5 carbon atoms with a substituent independently selected
 at each occurrence from the group C₁₋₆ alkyl, C₃₋₆
 cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro,
 -OR¹⁷, SH, -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸,
 -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CONR¹⁷R¹⁹, -NR¹⁵CO₂R¹⁸,
 10 -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and each heteroaryl being
 substituted on any nitrogen atom with 0-1 substituents
 selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and
 SO₂R^{14a}; and,
- 15 provided that when D is imidazole or triazole, R¹ is other
 than unsubstituted C₁₋₆ linear or branched alkyl or
 C₃₋₆ cycloalkyl.

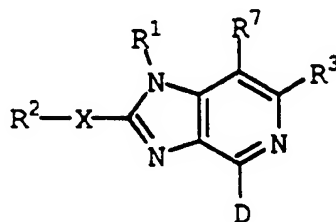
- 20 2. A compound according to Claim 1, wherein the compound
 is of formula Ia:



(Ia).

25

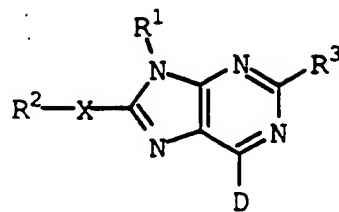
3. A compound according to Claim 1, wherein the compound
 is of formula Ib:



30

(Ib).

4. A compound according to Claim 1, wherein the compound
 5 is of formula Ic:

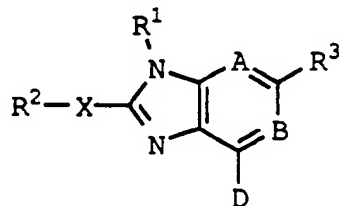


(Ic).

10

5. A pharmaceutical composition, comprising: a
 pharmaceutically acceptable carrier and a
 therapeutically effective amount of a compound of
 formula (I):

15



(I)

or a stereoisomer or pharmaceutically acceptable salt form
 thereof, wherein:

20

A is N or C-R⁷;

B is N or C-R⁸;

25

provided that at least one of the groups A and B is N;

D is an aryl or heteroaryl group attached through an
 unsaturated carbon atom;

X is selected from the group CH-R⁹, N-R¹⁰, O, S(O)_n and a bond;

n is 0, 1 or 2;

5

R¹ is selected from the group C₁₋₁₀ alkyl, C₂₋₁₀ alkenyl, C₂₋₁₀ alkynyl, C₃₋₈ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, -SO₂-C₁₋₁₀ alkyl, -SO₂-R^{1a}, and -SO₂-R^{1b};

10

R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b}, -CONR^{13a}R^{16a}, 1-morpholinyl, 1-piperidinyl, 15 1-piperazinyl, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-, and wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents 20 selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

20

R¹ is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, 25 R^{1c}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₄ alkoxy-C₁₋₄ alkyl, and C₃₋₈ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

30

provided that R¹ is other than:

- (a) a 3-cyclopropyl-3-methoxypropyl group;
- (b) an unsubstituted-(alkoxy)methyl group; and,
- (c) a 1-hydroxyalkyl group;

35

also provided that when R¹ alkyl substituted with OH, then the carbon adjacent to the ring N is other than CH₂;

R^{1a} is aryl and is selected from the group phenyl, naphthyl, indanyl and indenyl, each R^{1a} being substituted with 0-5 substituents independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH, -S(O)_nR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂, -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a};

R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-onyl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH, -S(O)_mR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂, -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a} and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

R^{1c} is heterocyclyl and is a saturated or partially saturated heteroaryl, each heterocyclyl being substituted on 0-4 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR^{13a}, SH, -S(O)_nR^{14b}, -COR^{13a},

-OC(O)R^{14b}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a},
-NR^{15a}CO₂R^{14b}, -NR^{13a}R^{16a}, and -CONR^{13a}R^{16a} and each
heterocyclyl being substituted on any nitrogen atom
with 0-1 substituents selected from the group R^{13a},
5 CO₂R^{14b}, COR^{14b} and SO₂R^{14b} and wherein any sulfur atom
is optionally monooxidized or dioxidized;

R² is selected from the group C₁₋₄ alkyl, C₃₋₈ cycloalkyl,
C₂₋₄ alkenyl, and C₂₋₄ alkynyl and is substituted with
10 0-3 substituents selected from the group -CN, hydroxy,
halo and C₁₋₄ alkoxy;

alternatively R², in the case where X is a bond, is selected
from the group -CN, CF₃ and C₂F₅;

15 R³, R⁷ and R⁸ are independently selected at each occurrence
from the group H, Br, Cl, F, I, -CN, C₁₋₄ alkyl, C₃₋₈
cycloalkyl, C₁₋₄ alkoxy, C₁₋₄ alkylthio, C₁₋₄
alkylsulfinyl, C₁₋₄ alkylsulfonyl, amino, C₁₋₄
20 alkylamino, (C₁₋₄ alkyl)₂amino and phenyl, each phenyl
is substituted with 0-3 groups selected from the group
C₁₋₇ alkyl, C₃₋₈ cycloalkyl, Br, Cl, F, I, C₁₋₄
haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, C₁₋₄
alkylthio, C₁₋₄ alkyl sulfinyl, C₁₋₄ alkylsulfonyl, C₁₋₆
25 alkylamino and (C₁₋₄ alkyl)₂amino;

provided that when R¹ is unsubstituted C₁₋₁₀ alkyl, then R³
is other than substituted or unsubstituted phenyl;

30 R⁹ and R¹⁰ are independently selected at each occurrence
from the group H, C₁₋₄ alkyl, C₃₋₆ cycloalkyl-C₁₋₄ alkyl
and C₃₋₈ cycloalkyl;

35 R¹³ is selected from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl,
C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆
cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-,
heteroaryl and heteroaryl(C₁₋₄ alkyl)-;

R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)- and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy C₁₋₄ haloalkoxy, and dimethylamino;

R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

R¹⁷ is selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₁₋₄ haloalkyl, R¹⁴S(O)_n-C₁₋₄ alkyl, and R^{17b}R^{19b}N-C₂₋₄ alkyl;

R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;

alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;

alternatively, in an NR^{17b}R^{19b} moiety, R^{17b} and R^{19b} taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R¹³, CO₂R¹⁴, COR¹⁴ and SO₂R¹⁴;

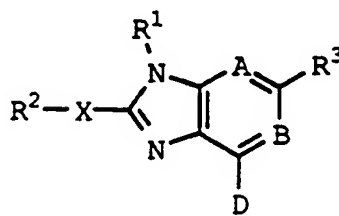
R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and C₁₋₄ haloalkyl;

aryl is independently selected at each occurrence from the group phenyl, naphthyl, indanyl and indenyl, each aryl being substituted with 0-5 substituents independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, methylenedioxy, C₁₋₄ alkoxy-C₁₋₄ alkoxy, -OR¹⁷, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, -NO₂, SH, -S(O)_nR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CONR¹⁷R¹⁹, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and up to 1 phenyl, each phenyl substituent being substituted with 0-4 substituents selected from

the group C₁₋₃ alkyl, C₁₋₃ alkoxy, Br, Cl, F, I, -CN, dimethylamino, CF₃, C₂F₅, OCF₃, SO₂Me and acetyl; and,

- heteroaryl is independently selected at each occurrence from
- 5 the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, triazolyl, tetrazolyl, indazolyl,
- 10 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide, 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 0-4
- 15 carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH, -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸, -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CONR¹⁷R¹⁹, -NR¹⁵CO₂R¹⁸,
- 20 -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and SO₂R^{14a}.
- 25 6. A method of treating affective disorder, anxiety, depression, headache, irritable bowel syndrome, post-traumatic stress disorder, supranuclear palsy, immune suppression, Alzheimer's disease, gastrointestinal diseases, anorexia nervosa or other feeding disorder,
- 30 drug addiction, drug or alcohol withdrawal symptoms, inflammatory diseases, cardiovascular or heart-related diseases, fertility problems, human immunodeficiency virus infections, hemorrhagic stress, obesity, infertility, head and spinal cord traumas, epilepsy,
- 35 stroke, ulcers, amyotrophic lateral sclerosis, hypoglycemia or a disorder the treatment of which can be effected or facilitated by antagonizing CRF, including

but not limited to disorders induced or facilitated by CRF, in mammals, comprising: administering to the mammal a therapeutically effective amount of a compound of formula (I):



(I)

10 or a stereoisomer or pharmaceutically acceptable salt form thereof, wherein:

A is N or C-R⁷;

B is N or C-R⁸;

15

provided that at least one of the groups A and B is N;

D is an aryl or heteroaryl group attached through an unsaturated carbon atom;

20

X is selected from the group CH-R⁹, N-R¹⁰, O, S(O)_n and a bond;

n is 0, 1 or 2;

25

R¹ is selected from the group C₁₋₁₀ alkyl, C₂₋₁₀ alkenyl, C₂₋₁₀ alkynyl, C₃₋₈ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, -SO₂-C₁₋₁₀ alkyl, -SO₂-R^{1a}, and -SO₂-R^{1b};

30

R¹ is substituted with 0-1 substituents selected from the group -CN, -S(O)_nR^{14b}, -COR^{13a}, -CO₂R^{13a}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a}, -NR^{15a}CO₂R^{14b}, -CONR^{13a}R^{16a}, 1-morpholinyl, 1-piperidinyl,

1-piperazinyl, and C₃₋₈ cycloalkyl, wherein 0-1 carbon atoms in the C₄₋₈ cycloalkyl is replaced by a group selected from the group -O-, -S(O)_n-, -NR^{13a}-, -NCO₂R^{14b}-, -NCOR^{14b}- and -NSO₂R^{14b}-, and wherein N₄ in 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

R¹ is also substituted with 0-3 substituents independently selected at each occurrence from the group R^{1a}, R^{1b}, R^{1c}, C₁₋₆ alkyl, C₂₋₈ alkenyl, C₂₋₈ alkynyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -OR^{13a}, -NR^{13a}R^{16a}, C₁₋₄ alkoxy-C₁₋₄ alkyl, and C₃₋₈ cycloalkyl which is substituted with 0-1 R⁹ and in which 0-1 carbons of C₄₋₈ cycloalkyl is replaced by -O-;

provided that R¹ is other than:

- (a) a 3-cyclopropyl-3-methoxypropyl group;
- (b) an unsubstituted-(alkoxy)methyl group; and,
- (c) a 1-hydroxyalkyl group;

also provided that when R¹ alkyl substituted with OH, then the carbon adjacent to the ring N is other than CH₂;

R^{1a} is aryl and is selected from the group phenyl, naphthyl, indanyl and indenyl, each R^{1a} being substituted with 0-5 substituents independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH, -S(O)_nR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂, -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and -CONR^{17a}R^{19a};

R^{1b} is heteroaryl and is selected from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl, thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl,

benzothienyl, benzothiazolyl, benzoxazolyl,
 isoxazolyl, pyrazolyl, triazolyl, tetrazolyl,
 indazolyl, 2,3-dihydrobenzofuranyl,
 2,3-dihydrobenzothienyl,
 5 2,3-dihydrobenzothienyl-S-oxide,
 2,3-dihydrobenzothienyl-S-dioxide, indoliny, l,
 benzoxazolin-2-onyl, benzodioxolanyl and benzodioxane,
 each heteroaryl being substituted on 0-4 carbon atoms
 with a substituent independently selected at each
 10 occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl,
 Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH,
 -S(O)_mR¹⁸, -COR¹⁷, -OC(O)R¹⁸, -NR^{15a}COR¹⁷, -N(COR¹⁷)₂,
 -NR^{15a}CONR^{17a}R^{19a}, -NR^{15a}CO₂R¹⁸, -NR^{17a}R^{19a}, and
 -CONR^{17a}R^{19a} and each heteroaryl being substituted on
 15 any nitrogen atom with 0-1 substituents selected from
 the group R^{15a}, CO₂R^{14b}, COR^{14b} and SO₂R^{14b};

R^{1c} is heterocyclyl and is a saturated or partially
 saturated heteroaryl, each heterocyclyl being
 20 substituted on 0-4 carbon atoms with a substituent
 independently selected at each occurrence from the
 group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄
 haloalkyl, -CN, nitro, -OR^{13a}, SH, -S(O)_nR^{14b}, -COR^{13a},
 -OC(O)R^{14b}, -NR^{15a}COR^{13a}, -N(COR^{13a})₂, -NR^{15a}CONR^{13a}R^{16a},
 25 -NR^{15a}CO₂R^{14b}, -NR^{13a}R^{16a}, and -CONR^{13a}R^{16a} and each
 heterocyclyl being substituted on any nitrogen atom
 with 0-1 substituents selected from the group R^{13a},
 CO₂R^{14b}, COR^{14b} and SO₂R^{14b} and wherein any sulfur atom
 is optionally monooxidized or dioxidized;

30 R² is selected from the group C₁₋₄ alkyl, C₃₋₈ cycloalkyl,
 C₂₋₄ alkenyl, and C₂₋₄ alkynyl and is substituted with
 0-3 substituents selected from the group -CN, hydroxy,
 halo and C₁₋₄ alkoxy;

35 alternatively R², in the case where X is a bond, is selected
 from the group -CN, CF₃ and C₂F₅;

R³, R⁷ and R⁸ are independently selected at each occurrence from the group H, Br, Cl, F, I, -CN, C₁₋₄ alkyl, C₃₋₈ cycloalkyl, C₁₋₄ alkoxy, C₁₋₄ alkylthio, C₁₋₄ alkylsulfinyl, C₁₋₄ alkylsulfonyl, amino, C₁₋₄ alkylamino, (C₁₋₄ alkyl)₂amino and phenyl, each phenyl is substituted with 0-3 groups selected from the group C₁₋₇ alkyl, C₃₋₈ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, C₁₋₄ alkylthio, C₁₋₄ alkyl sulfinyl, C₁₋₄ alkylsulfonyl, C₁₋₆ alkylamino and (C₁₋₄ alkyl)₂amino;

provided that when R¹ is unsubstituted C₁₋₁₀ alkyl, then R³ is other than substituted or unsubstituted phenyl;

R⁹ and R¹⁰ are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₆ cycloalkyl-C₁₋₄ alkyl and C₃₋₈ cycloalkyl;

R¹³ is selected from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)-;

R^{13a} and R^{16a} are independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

R¹⁴ is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, aryl, aryl(C₁₋₄ alkyl)-, heteroaryl and heteroaryl(C₁₋₄ alkyl)- and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy C₁₋₄ haloalkoxy, and dimethylamino;

R^{14a} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl and benzyl, each benzyl being substituted on the aryl moiety with 0-1 substituents selected from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

R^{14b} is selected from the group C₁₋₄ alkyl, C₁₋₄ haloalkyl, C₁₋₄ alkoxy-C₁₋₄ alkyl, C₃₋₆ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

R¹⁵ is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, phenyl and benzyl, each phenyl or benzyl being substituted on the aryl moiety with 0-3 groups chosen from the group C₁₋₄ alkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, nitro, C₁₋₄ alkoxy, C₁₋₄ haloalkoxy, and dimethylamino;

R^{15a} is independently selected at each occurrence from the group H, C₁₋₄ alkyl, C₃₋₇ cycloalkyl, and C₃₋₆ cycloalkyl-C₁₋₆ alkyl;

R¹⁷ is selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, C₁₋₄ haloalkyl, R¹⁴S(O)_n-C₁₋₄ alkyl, and R^{17b}R^{19b}N-C₂₋₄ alkyl;

R¹⁸ and R¹⁹ are independently selected at each occurrence from the group H, C₁₋₆ alkyl, C₃₋₁₀ cycloalkyl, C₃₋₆ cycloalkyl-C₁₋₆ alkyl, C₁₋₂ alkoxy-C₁₋₂ alkyl, and C₁₋₄ haloalkyl;

alternatively, in an NR¹⁷R¹⁹ moiety, R¹⁷ and R¹⁹ taken together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N₄ in

1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13} , CO_2R^{14} , COR^{14} and SO_2R^{14} ;

- alternatively, in an $NR^{17b}R^{19b}$ moiety, R^{17b} and R^{19b} taken
 5 together form 1-pyrrolidinyl, 1-morpholinyl, 1-piperidinyl or 1-piperazinyl, wherein N_4 in 1-piperazinyl is substituted with 0-1 substituents selected from the group R^{13} , CO_2R^{14} , COR^{14} and SO_2R^{14} ;
- 10 R^{17a} and R^{19a} are independently selected at each occurrence from the group H, C_{1-6} alkyl, C_{3-10} cycloalkyl, C_{3-6} cycloalkyl- C_{1-6} alkyl and C_{1-4} haloalkyl;
- aryl is independently selected at each occurrence from the
 15 group phenyl, naphthyl, indanyl and indenyl, each aryl being substituted with 0-5 substituents independently selected at each occurrence from the group C_{1-6} alkyl, C_{3-6} cycloalkyl, methylenedioxy, C_{1-4} alkoxy- C_{1-4} alkoxy, $-OR^{17}$, Br, Cl, F, I, C_{1-4} haloalkyl, $-CN$, $-NO_2$,
 20 SH, $-S(O)_nR^{18}$, $-COR^{17}$, $-CO_2R^{17}$, $-OC(O)R^{18}$, $-NR^{15}COR^{17}$, $-N(COR^{17})_2$, $-NR^{15}CONR^{17}R^{19}$, $-NR^{15}CO_2R^{18}$, $-NR^{17}R^{19}$, and $-CONR^{17}R^{19}$ and up to 1 phenyl, each phenyl substituent being substituted with 0-4 substituents selected from the group C_{1-3} alkyl, C_{1-3} alkoxy, Br, Cl, F, I, $-CN$,
 25 dimethylamino, CF_3 , C_2F_5 , OCF_3 , SO_2Me and acetyl; and,

- heteroaryl is independently selected at each occurrence from the group pyridyl, pyrimidinyl, triazinyl, furanyl, quinolinyl, isoquinolinyl, thienyl, imidazolyl,
 30 thiazolyl, indolyl, pyrrolyl, oxazolyl, benzofuranyl, benzothienyl, benzothiazolyl, benzoxazolyl, isoxazolyl, triazolyl, tetrazolyl, indazolyl, 2,3-dihydrobenzofuranyl, 2,3-dihydrobenzothienyl, 2,3-dihydrobenzothienyl-S-oxide,
 35 2,3-dihydrobenzothienyl-S-dioxide, indolinyl, benzoxazolin-2-on-yl, benzodioxolanyl and benzodioxane, each heteroaryl being substituted 0-4

carbon atoms with a substituent independently selected at each occurrence from the group C₁₋₆ alkyl, C₃₋₆ cycloalkyl, Br, Cl, F, I, C₁₋₄ haloalkyl, -CN, nitro, -OR¹⁷, SH, -S(O)_mR¹⁸, -COR¹⁷, -CO₂R¹⁷, -OC(O)R¹⁸,
5 -NR¹⁵COR¹⁷, -N(COR¹⁷)₂, -NR¹⁵CONR¹⁷R¹⁹, -NR¹⁵CO₂R¹⁸, -NR¹⁷R¹⁹, and -CONR¹⁷R¹⁹ and each heteroaryl being substituted on any nitrogen atom with 0-1 substituents selected from the group R¹⁵, CO₂R^{14a}, COR^{14a} and SO₂R^{14a}.

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INTERNATIONAL SEARCH REPORT

International Application No

PCT/US 98/13913

A. CLASSIFICATION OF SUBJECT MATTER

IPC 6 C07D471/04 C07D473/00 A61K31/505 A61K31/535
 //(C07D471/04,235:00,221:00)

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 6 C07D A61K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|----------|---|-----------------------|
| A | EP 0 773 023 A (PFIZER INC.) 14 May 1997 see claims | 1-6 |
| A | WO 95 10506 A (THE DU PONT MERCK PHARMACEUTICAL COMPANY) 20 April 1995 cited in the application see claims | 1-6 |
| A | WO 95 34563 A (PFIZER INC.) 21 December 1995 cited in the application see claims | 1-6 |
| A | WO 95 33750 A (PFIZER INC.) 14 December 1995 cited in the application see claims | 1-6 |
| -/-- | | |



Further documents are listed in the continuation of box C.



Patent family members are listed in annex.

* Special categories of cited documents:

- "A" document defining the general state of the art which is not considered to be of particular relevance
- "E" earlier document but published on or after the international filing date
- "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- "O" document referring to an oral disclosure, use, exhibition or other means
- "P" document published prior to the international filing date but later than the priority date claimed

- "T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
- "X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
- "Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.
- "G" document member of the same patent family

Date of the actual completion of the international search

20 October 1998

Date of mailing of the international search report

30/10/1998

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INTERNATIONAL SEARCH REPORT

Int. Appl. No.

PCT/US 98/13913

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

| Category | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|----------|--|-----------------------|
| P,A | EP 0 812 831 A (PFIZER INC.) 17 December 1997 see claims --- | 1-6 |
| P,A | WO 98 08847 A (PFIZER INC.) 5 March 1998 see claims ----- | 1-6 |

INTERNATIONAL SEARCH REPORT

national application No.

PCT/US 98/ 13913

Box I Observations where certain claims were found uns archable (C ntinuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☒ Claims Nos.: 6
because they relate to subject matter not required to be searched by this Authority, namely:
Remark: Although claim 6
is directed to a method of treatment of the human/animal
body, the search has been carried out and based on the alleged
effects of the compound/composition.
2. ☐ Claims Nos.:
because they relate to parts of the International Application that do not comply with the prescribed requirements to such
an extent that no meaningful International Search can be carried out, specifically:
3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all
searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment
of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report
covers only those claims for which fees were paid, specifically claims Nos.:
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is
restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.
- ☐ No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/US 98/13913

| Patent document cited in search report | Publication date | Patent family member(s) | Publication date |
|---|---------------------|--|--|
| EP 773023 A | 14-05-1997 | CA 2189830 A JP 9132528 A | 09-05-1997 20-05-1997 |
| WO 9510506 A | 20-04-1995 | AU 692484 B AU 8012294 A BR 9407799 A CA 2174080 A CN 1142817 A CZ 9601014 A EP 0723533 A FI 961599 A HR 940664 A HU 74464 A JP 9504520 T NO 961425 A NZ 274978 A PL 313973 A SK 47096 A ZA 9407921 A | 11-06-1998 04-05-1995 06-05-1997 20-04-1995 12-02-1997 13-11-1996 31-07-1996 07-06-1996 31-12-1996 30-12-1996 06-05-1997 12-06-1996 27-04-1998 05-08-1996 01-10-1996 11-04-1996 |
| WO 9534563 A | 21-12-1995 | AU 687196 B AU 2350595 A BR 9502707 A CA 2192820 A CN 1150803 A CZ 9603670 A EP 0765327 A FI 965022 A HU 75776 A JP 9507855 T NO 965378 A PL 317705 A | 19-02-1998 05-01-1996 04-06-1996 21-12-1995 28-05-1997 15-10-1997 02-04-1997 13-12-1996 28-05-1997 12-08-1997 13-12-1996 28-04-1997 |
| WO 9533750 A | 14-12-1995 | AU 692548 B AU 2453095 A BR 9502708 A CA 2192354 A CN 1150428 A EP 0764166 A FI 964894 A | 11-06-1998 04-01-1996 30-04-1996 14-12-1995 21-05-1997 26-03-1997 05-12-1996 |

INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/US 98/13913

| Patent document cited in search report | Publication date | Patent family member(s) | Publication date |
|---|---------------------|----------------------------|---------------------|
| WO 9533750 A | | HR 950321 A | 28-02-1998 |
| | | HU 75774 A | 28-05-1997 |
| | | JP 9507249 T | 22-07-1997 |
| | | NO 965237 A | 06-02-1997 |
| | | NZ 285442 A | 27-05-1998 |
| | | PL 320631 A | 13-10-1997 |
| EP 812831 A | 17-12-1997 | CA 2207348 A | 11-12-1997 |
| | | JP 10072449 A | 17-03-1998 |
| WO 9808847 A | 05-03-1998 | AU 3456197 A | 19-03-1998 |

